Atmosphere Monitoring

Satellite data assimilation of atmospheric composition

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Why atmospheric composition at an operational weather prediction centre?

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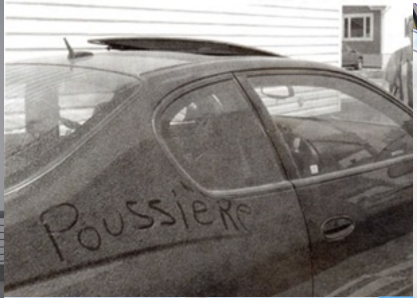
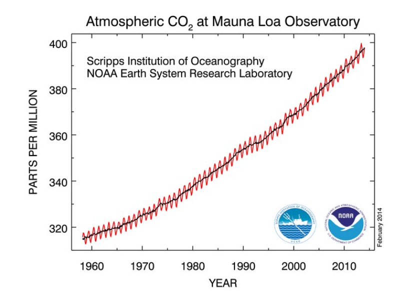
- Poor air quality is a major public health issue in many countries.
- Local authorities need accurate and timely information to implement effective air pollution mitigation measures.
- Accurate air quality forecasts require accurate transport models.
- Can leverage sophisticated data acquisition infrastructures implemented at operational weather prediction centers.
- Atmospheric composition also impacts the weather and forecasts.





Why this lecture?

- Basic data assimilation theory is the same for atmospheric composition, but…
  - Radiance assimilation is not always feasible (yet)
  - Atmospheric composition data assimilation is much more influenced by additional factors such as emissions and chemistry than by the initial values
  - With many species not being observed, the problem is even more underdetermined than the standard NWP case
- Atmospheric composition impacts the basic NWP problem as well

Atmosphere Monitoring

1. Copernicus Atmosphere Monitoring Service (CAMS)

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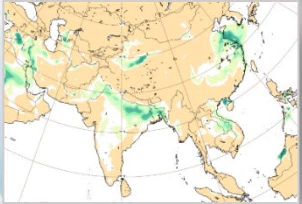
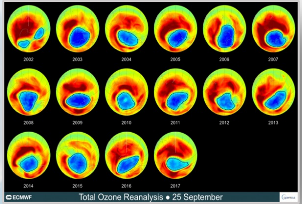
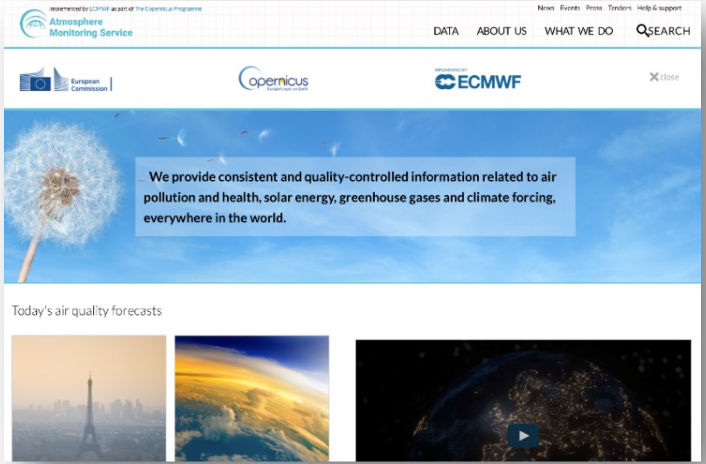
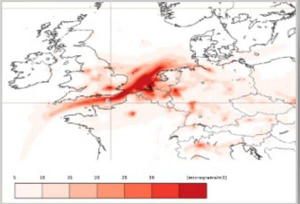
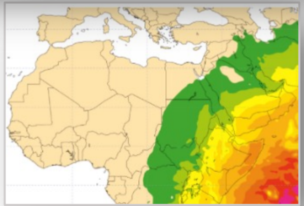
What the Copernicus Atmosphere Monitoring Service has to offer











The CAMS portfolio includes Earth Observation based information products about:

- global atmospheric composition;
- the ozone layer;
- air quality in Europe;
- emissions and surface fluxes of key pollutants and greenhouse gases;
- solar radiation;
- climate radiative forcing.
- reanalysis of atmospheric composition (back to 2003)

Quarterly validation reports of global and regional outputs.

This is done by assimilating atmospheric composition data into the IFS (in addition to meteorological observations)

https://atmosphere.copernicus.eu

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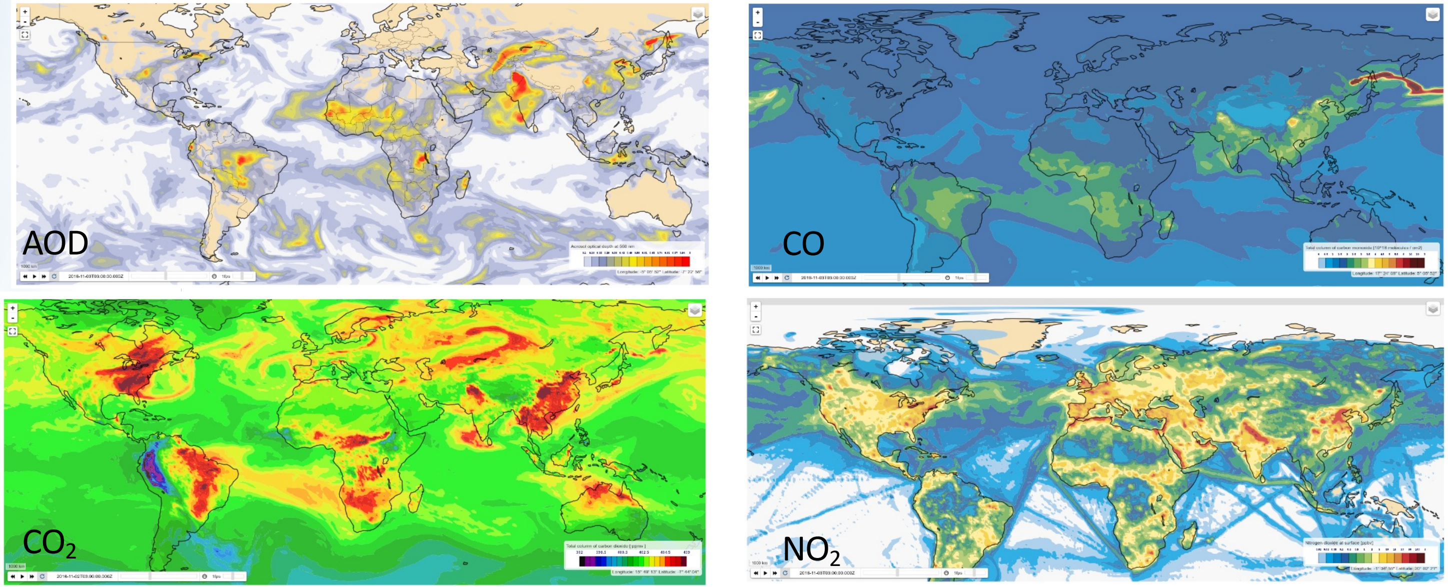
CAMS Global System



40km horizontal resolution at 137 model levels; two 5-day forecasts at 00z and 12z UTC each day

- **Aerosols (AOD and concentrations): e.g. biomass burning, dust, sea-salt, sulphate, …**
- **Reactive gases: CO, HCHO, NO_2, O_3, SO_2**

9km horizontal resolution at 137 model levels; one 5-day forecast per day (CO_2, CH_4, linear CO)

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2. Observations of atmospheric composition

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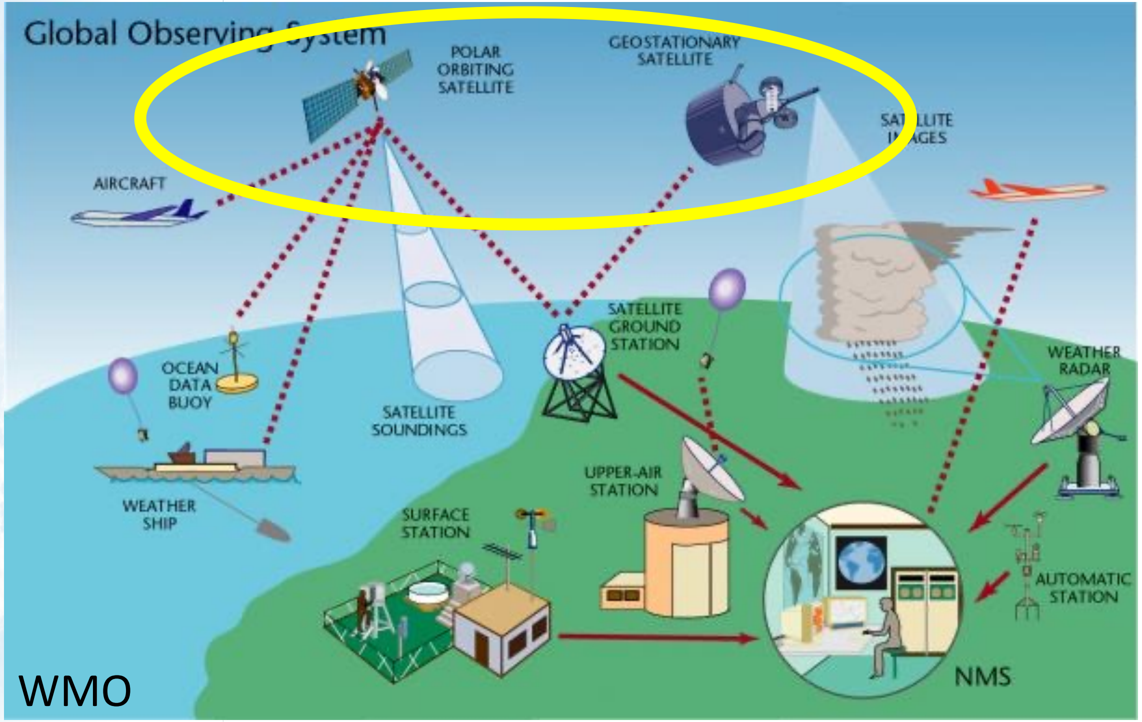
Global observing system



We want to provide information about near-surface air quality

- CAMS assimilates satellite retrievals of atmospheric composition
- CAMS uses ground-based & aircraft data and satellite retrievals for validation

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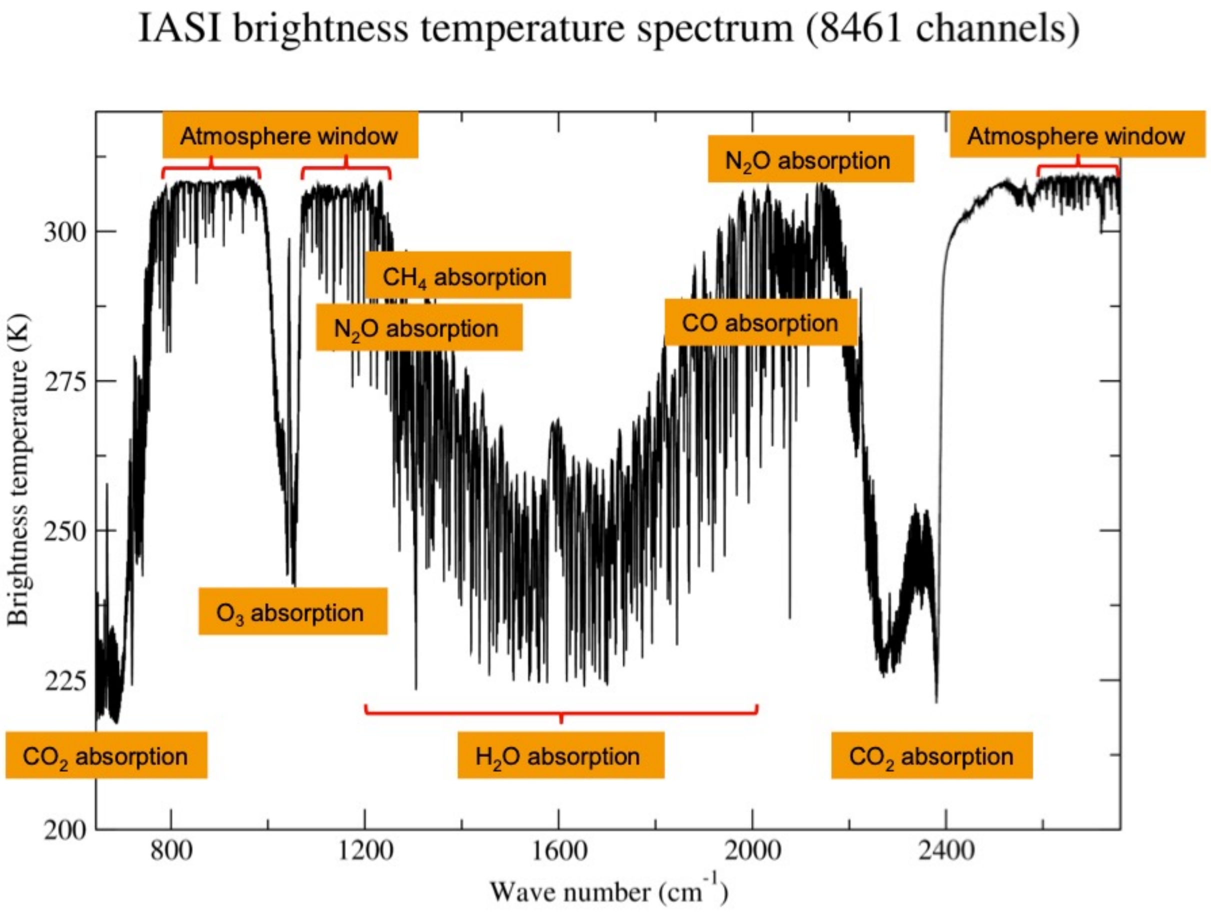
Spectral signature of trace gases



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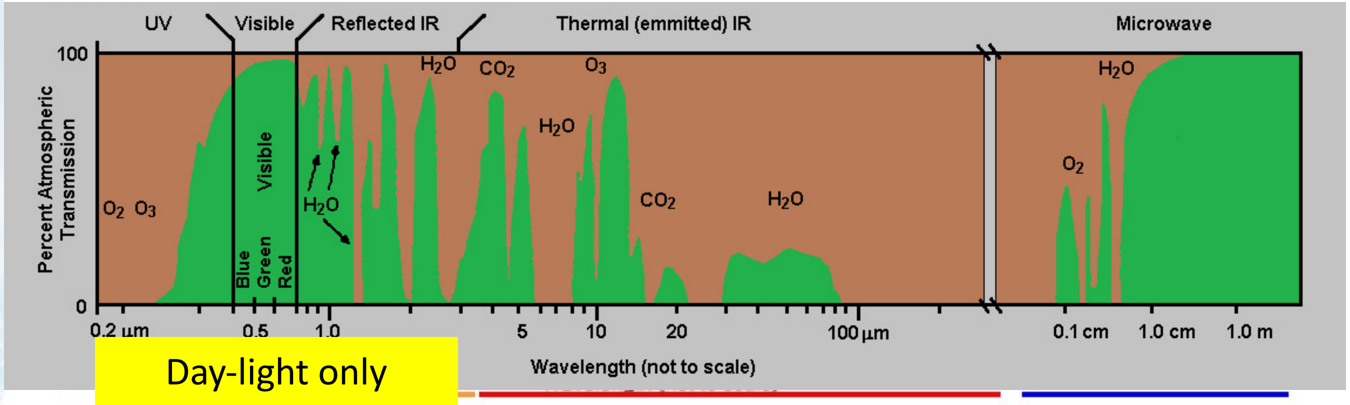
Spectral signature of trace gases

NIR, SWIR



O_3
H_2O
NO_2
SO_2
H_2CO, $C_2H_2O_2$
IO
BrO

AOD MODIS

GOME, GOME-2, SCIAMACHY,
OMI *at nadir* TROPOMI
SCIAMACHY, OSIRIS *at limb*

CO_2
CH_4
CO

SCIAMACHY,
GOSAT, OCO *at nadir* TROPOMI

H_2O
CO_2
CH_4
N_2O
O_3
CO
HNO_3
NH_3
CFC11, CFC12, …
CH_3OH, HCOOH, C_2H_2, C_2H_6,…
+ isotopologues

TES, AIRS, IASI, MOPITT *at nadir*
MIPAS, ACE *at limb*

O_2
H_2O, OH, HO_2
HNO_3
HCl, BrO, ClO, HOCl
O3
CO
HCN, CH_3CN

DMR, MLS *at limb*

Credit: M. Van Roozendael

Satellite observations

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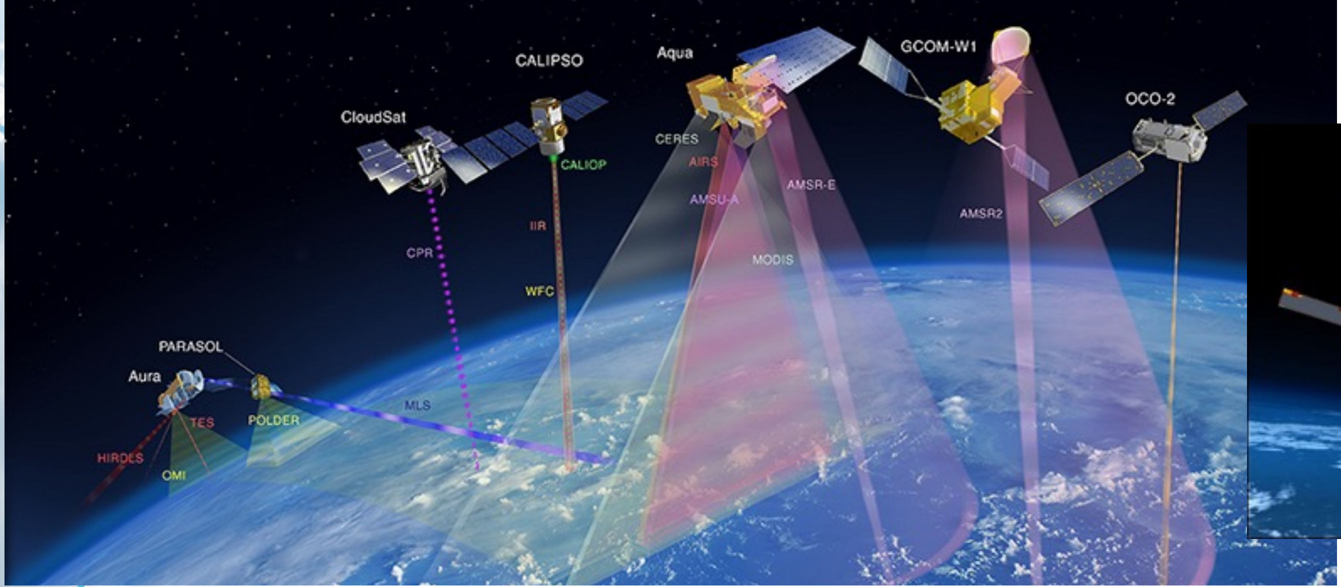
The American A-train has been very important



IASI & GOME-2 onboard the European MetOp satellites have also provided a wealth of atmospheric composition data.

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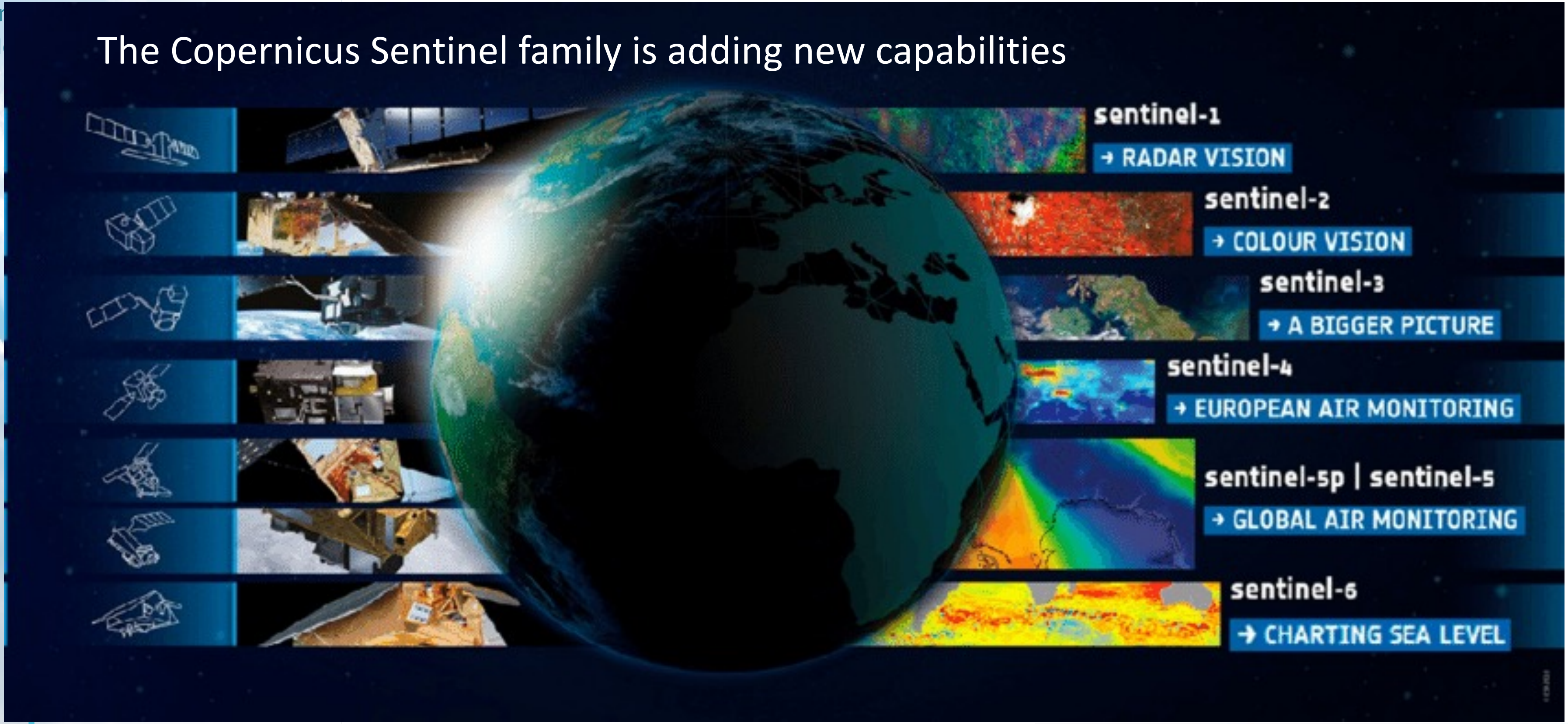
Satellite observations



AC Observations used in CAMS

	O_3				
Satellite	AURA		Metop BC	S-NPP & NOAA 20	Sentinel 5p
Instrument	MLS	OMI	GOME-2	OMPS	TropOMI
Type	Strat Profiles	Total Columns	Total Columns	Layers	Total Columns

	CO		
Satellite	Metop AB	TERRA	Sentinel 5p
Instrument	IASI	MOPITT	TropOMI
Type	Total Columns	Total Columns	Total Columns

	NO_2	
Satellite	Metop BC	Sentinel 5p
Instrument	GOME-2	TropOMI
Type	Tropospheric Columns	Tropospheric Columns

	SO_2	
Satellite	Metop BC	Sentinel 5p
Instrument	GOME-2	TropOMI
Type	Tropospheric Columns	Tropospheric Columns

	AOD			
Satellite	AQUA & TERRA	Metop BC	S-NPP & NOAA-20	Sentinel-3
Instrument	MODIS	PMAP	VIIRS	SLSTR
Type	AOD	AOD	AOD	AOD

	CH_4		
Satellite	GOSAT	Metop BC	Sentinel 5p
Instrument	TANSO	IASI	TropOMI
Type	Total Columns	Total Columns	Total Columns

	CO_2		
Satellite	GOSAT	Metop BC	OCO-2
Instrument	TANSO	IASI	OCO-2
Type	Total Columns	Total Columns	Total columns

Around 20 different data streams are operationally assimilated or monitored into IFS on top of the meteorological data streams.

AC Observations used in CAMS

	O_3					CO			NO_2		SO_2		AOD				CH_4			CO_2		
Satellite	AURA		Metop BC	S-NPP & NOAA 20	Sentinel 5p	Metop AB	TERRA	Sentinel 5p	Metop BC	Sentinel 5p	Metop BC	Sentinel 5p	AQUA & TERRA	Metop BC	S-NPP & NOAA-20	Sentinel-3	GOSAT	Metop BC	Sentinel 5p	GOSAT	Metop BC	OCO-2
Instrument	MLS	OMI	GOME-2	OMPS	TropOMI	IASI	MOPITT	TropO	GOM	TropO	GOM	TropO	MOD	PMA	VIIR	SLST	TANSO	IASI	TropOMI	TANSO	IASI	OCO-2
Type	Strat Profiles	Total Columns	Total Columns	Layers	Total Columns	Total Columns	Total Columns	Total Columns	Tropospheric Columns	Tropospheric Columns	Tropospheric Columns	Tropospheric Columns	AOD	AOD	AOD	AOD	Total Columns	Total Columns	Total Columns	Total Columns	Total Columns	Total columns

All from LEOs

Around 20 different data streams are operationally assimilated or monitored into IFS on top of the meteorological data streams.

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3. Radiances versus retrievals

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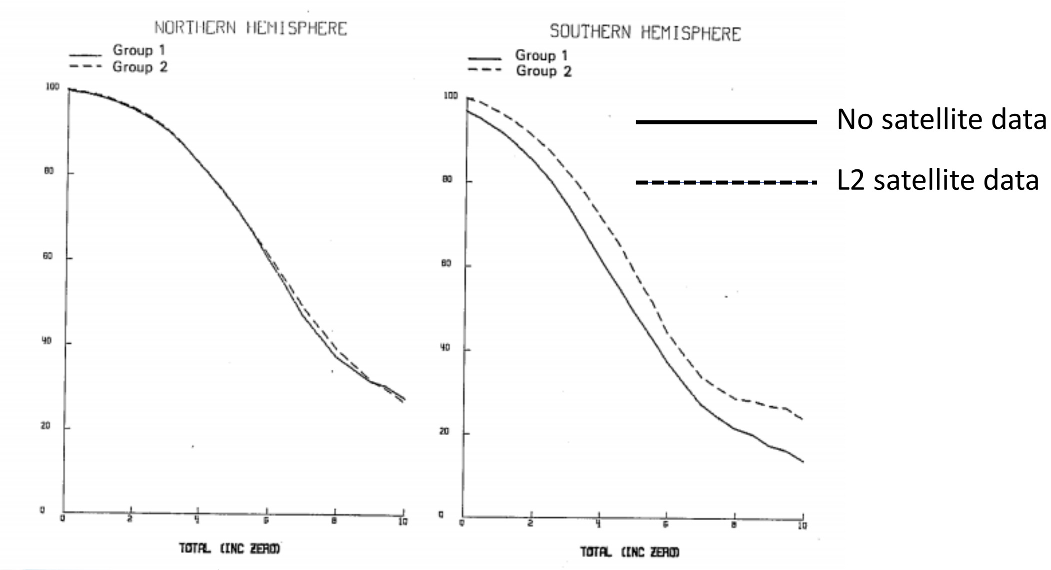
Use of retrievals in NWP – the 80s



Kelly and Pailleux, 1988

Assimilating temperature and water vapour satellite retrievals caused severe problems. Only after switch to radiance assimilation the real value of satellites was seen.

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Use of retrievals in NWP – the 80s

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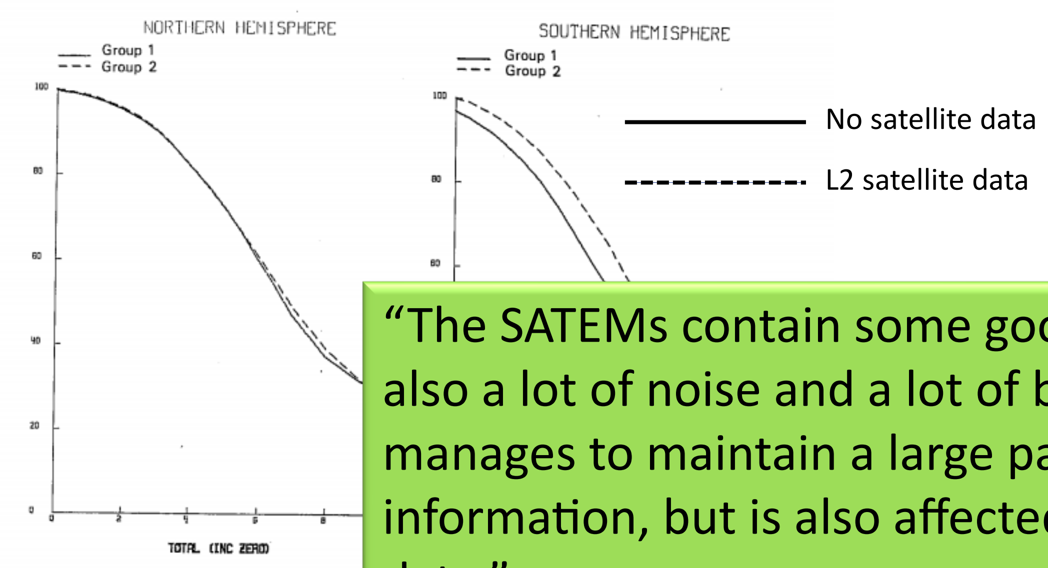

Kelly and Pailleux,

"The SATEMs contain some good information, but also a lot of noise and a lot of bad data. The analysis manages to maintain a large part of the good information, but is also affected by the poor quality data."

Assimilating temperature and water vapour satellite retrievals caused severe problems. Only after switch to radiance assimilation the real value of satellites was seen.

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Radiances versus retrievals

L2 retrievals generally use same methodology as data assimilation - minimize a cost function that contains the observations and some a-priori constraint:

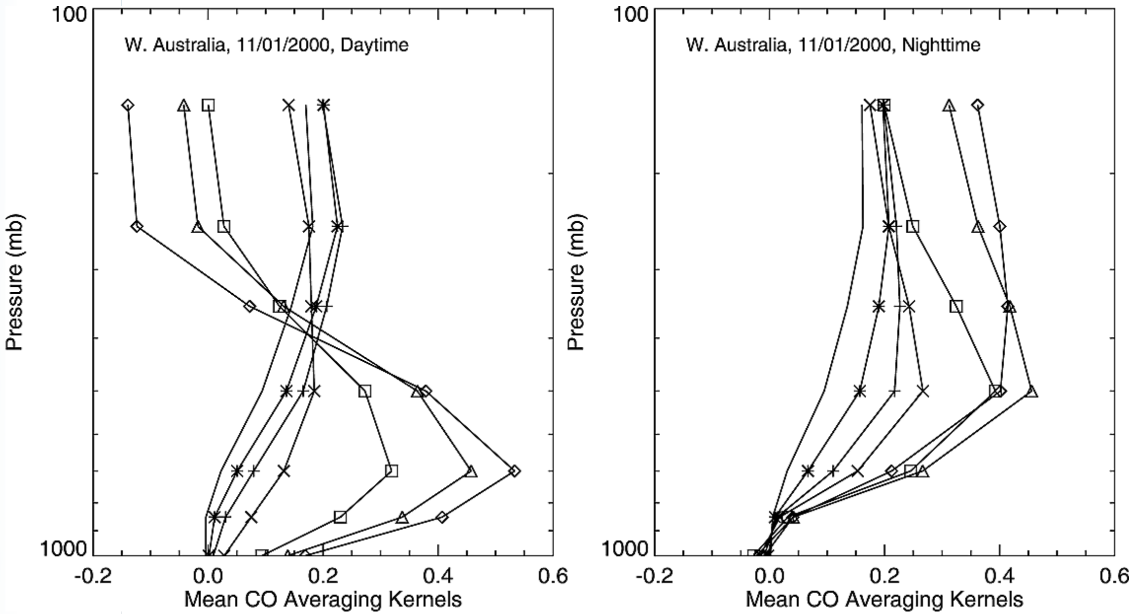
$$J(\mathbf{x}) = \frac{1}{2}(\mathbf{x} - \mathbf{x}_r^b)^{\mathrm{T}} \mathbf{B}_r^{-1} (\mathbf{x} - \mathbf{x}_r^b) + \frac{1}{2}[\mathbf{y}^o - H(\mathbf{x})]^{\mathrm{T}} \mathbf{R}^{-1} [\mathbf{y}^o - H(\mathbf{x})]$$

The retrieval equation: $\hat{x} = x_r^b + \mathbf{A}(x - x_r^b) + \boldsymbol{\varepsilon}$

The retrieved value will be biased relative to the assimilation model background, when the prior information is different from the model background.

This bias will have a vertical structure based on the vertical sensitivity of the observations. The averaging kernel **A** describes the vertical structure of the impact of the a priori information

Example MOPITT CO Averaging Kernels



From: Deeter et al. (2003) JGR

- Diurnal variations of Tsurf affect retrieval over land.
- CO near surface more detectable during day, AKs shift downwards
- Diurnal variability of AKs largest over e.g. deserts, smallest over sea
- If AKs are not used this can introduce an artificial diurnal CO cycle in the analysis

Assimilating retrievals: Column retrieval example

We can make use of the averaging kernel **A** in the observation:

$$d = y - H(\mathbf{x}_m) = \mathbf{x}_r^b + \mathbf{A}(\mathbf{x} - \mathbf{x}_r^b) + \varepsilon - H(\mathbf{x}_m)$$

Without averaging kernels in observation operator

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Assimilating retrievals: Column retrieval example

We can make use of the averaging kernel **A** in the observation:

$$d = y - H(\mathbf{x}_m) = \mathbf{x}_r^b + \mathbf{A}(\mathbf{x} - \mathbf{x}_r^b) + \varepsilon - H(\mathbf{x}_m)$$

Without averaging kernels in observation operator

$$d = y - \hat{H}(\mathbf{x}_m) = \mathbf{x}_r^b + \mathbf{A}(\mathbf{x} - \mathbf{x}_r^b) + \varepsilon - (\mathbf{x}_r^b + \mathbf{A}(H(\mathbf{x}_m) - \mathbf{x}_r^b))$$
$$= \mathbf{A}(\mathbf{x} - H(\mathbf{x}_m)) + \varepsilon$$

With averaging kernels in observation operator

We remove the influence of the a-priori profile if we use the averaging kernel to sample the model profile according to the assumptions made in the retrieval.

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Issues

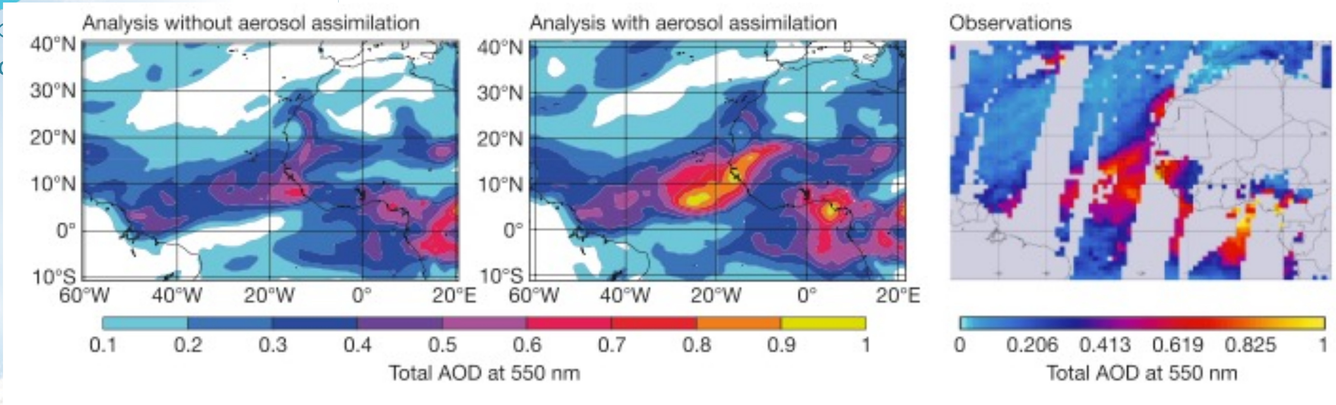
- Total column retrievals come with integrated averaging kernels; some information is lost
- Profile retrievals with full averaging kernels and retrieval errors can become difficult to handle
- Not all retrieval methods allow the estimation of an averaging kernel; e.g., neural networks
- Not all data providers use the same definition of averaging kernel in their data files
- Many different versions of the observation operator needed to deal with all variations
- We use:
    - Reactive gases: Profiles, columns with and without averaging kernels
    - Aerosols: Columns without averaging kernels, profiles being tested
    - Greenhouse gases: Radiances and columns with averaging kernels

Assimilating retrievals: summary

- Easier
- No radiative transfer model for some of the species of interest
- Bad experiences with radiance assimilation:

  Combination of model bias and VarBC in CO_2 data assimilation from AIRS and IASI radiances caused artificial long-term trend. Tests with IASI/AIRS ozone radiance assimilation led to degraded tropospheric ozone in CAMS
- Retrieval teams can focus their expertise fully on specific observation
- Good communication between data providers and data assimilation users needed
- Good characterization of retrieval is crucial
  - Averaging kernels
  - A priori
  - Error estimates
  - Quality flags

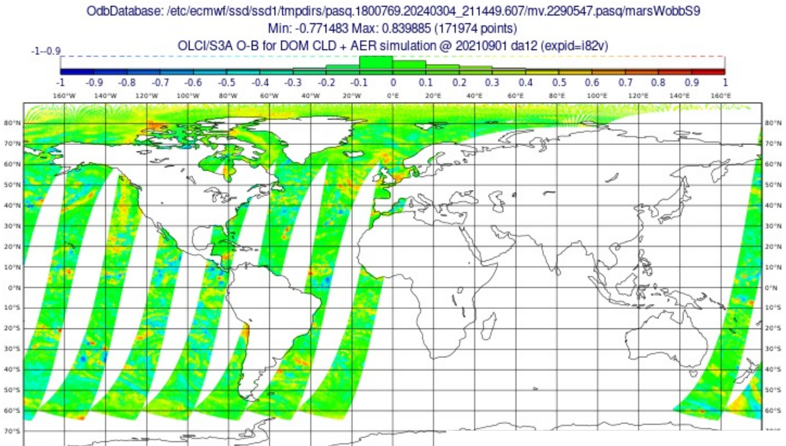
Current research



ARAS project

ARAS project used LUTs created from Oxford-RAL Aerosol and Cloud (ORAC) satellite retrieval scheme to replicate reflectances

CAMEO project will use RTTOV in the visible channels to replicate reflectances – capturing cloud and aerosols



CAMEO project

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4. Potential issues when assimilating AC satellite data

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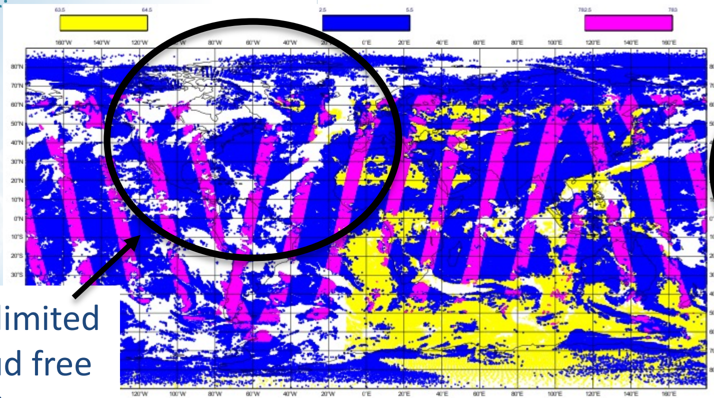
Example of satellite observation coverage

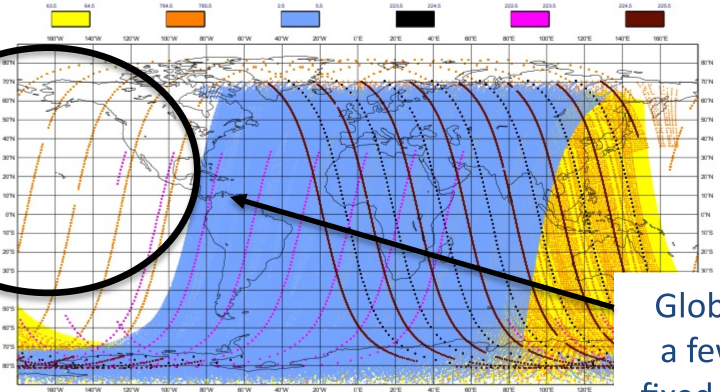
12-hour analysis cycle

CO: TROPOMI, MOPITT, IASI



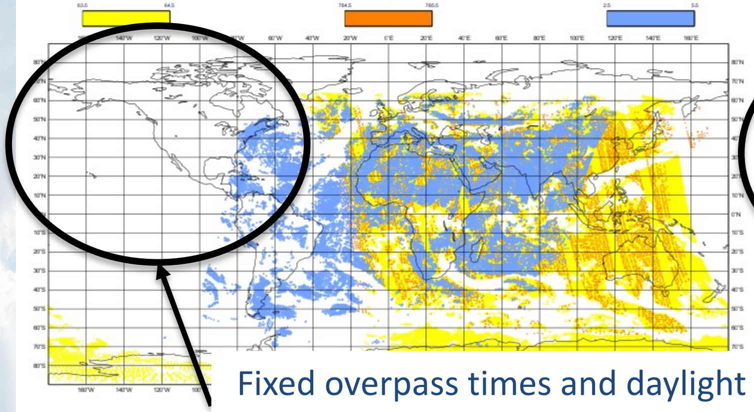
Often limited to cloud free conditions

O3: TROPOMI, GOME-2,OMI,SBUV,OMPS,MLS

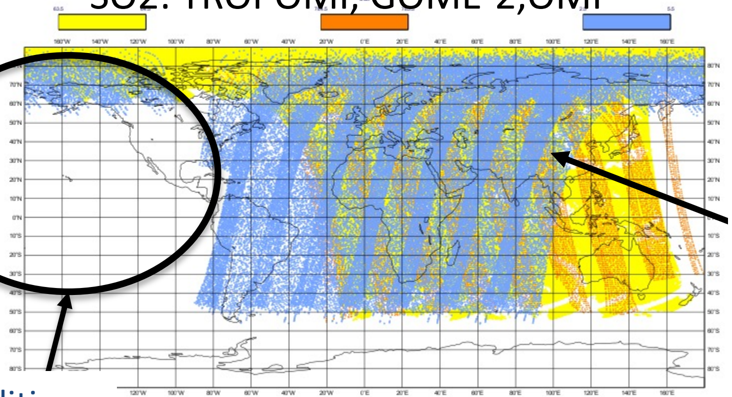


Global coverage in a few days (LEO) – fixed overpass time

NO2: TROPOMI, GOME-2,OMI



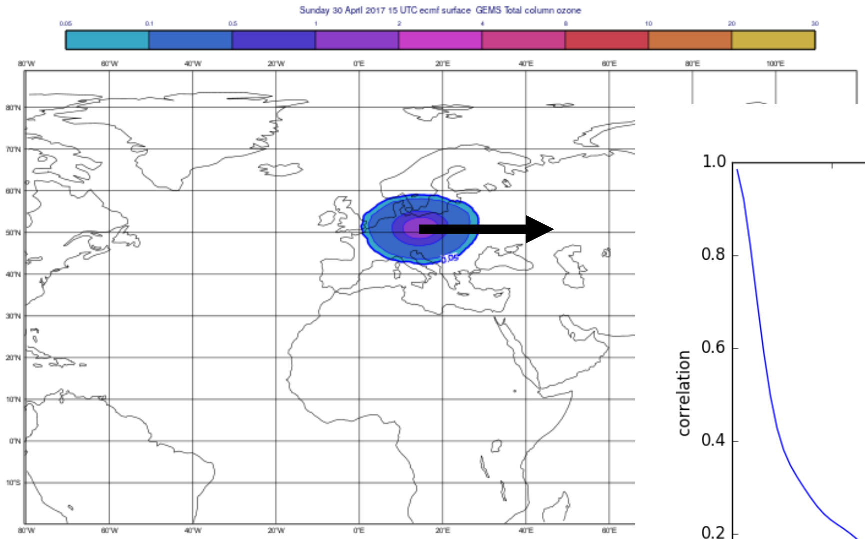
SO2: TROPOMI, GOME-2,OMI



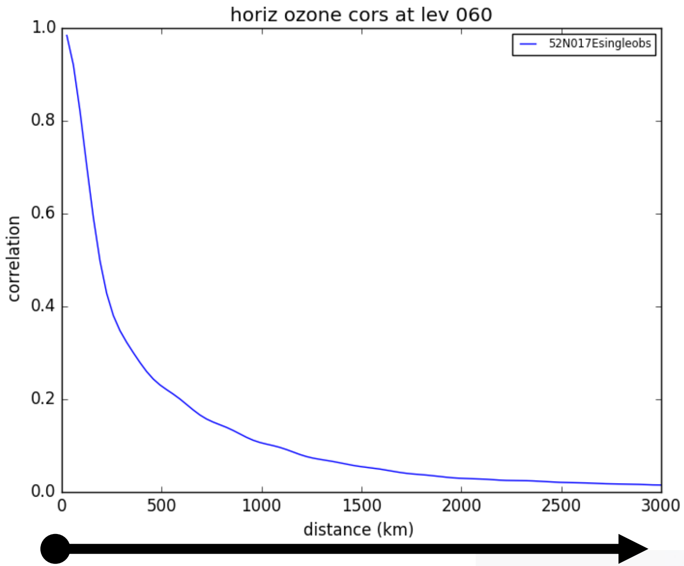
Total or tropospheric columns

Fixed overpass times and daylight conditions only (UV-VIS) -> no daily maximum/cycle

Increment from one TC ozone retrieval

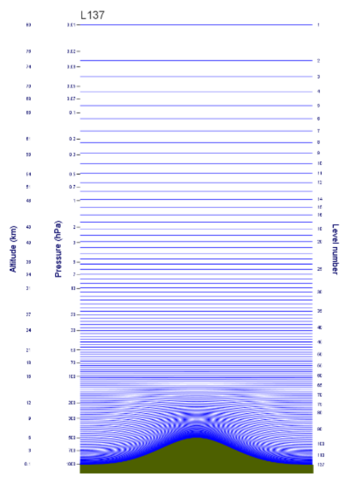


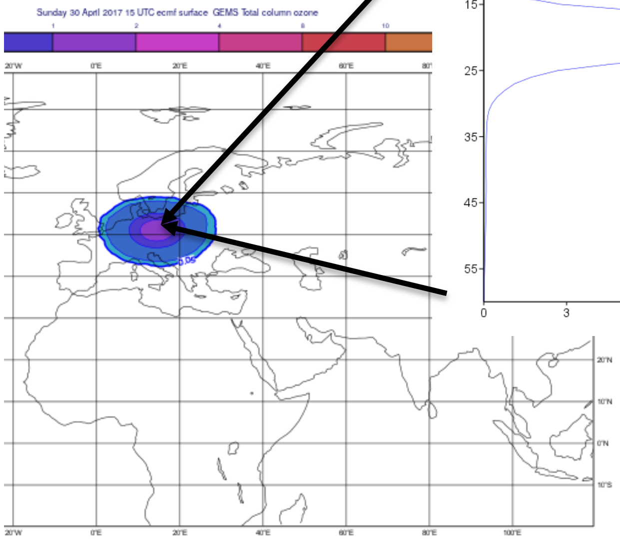
Increment created by a single ozone observation of 375 DU, 10 DU higher than background

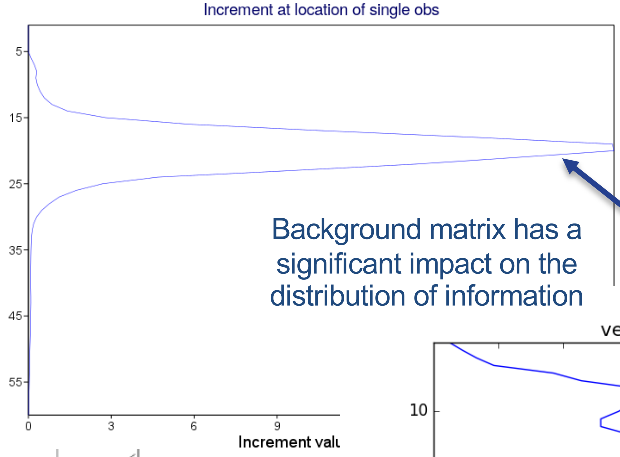


Horizontal correlation from the B-matrix that spreads the information from the single observation in the horizontal

Increment from one TC ozone retrieval



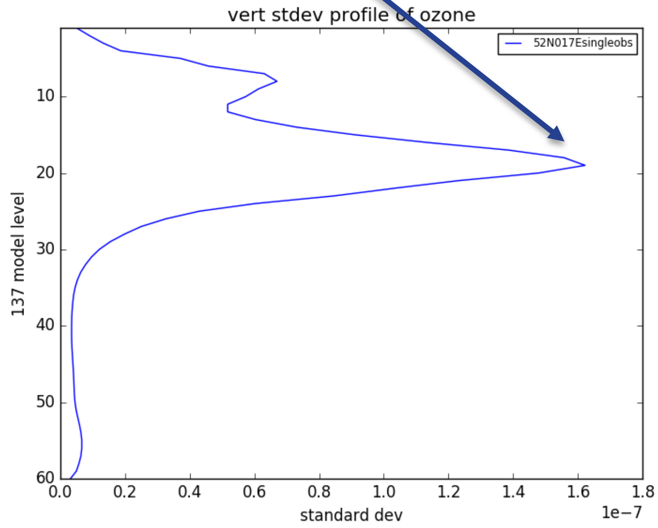




Vertical profile of the increment at the observation location

~35 hPa

Background matrix has a significant impact on the distribution of information



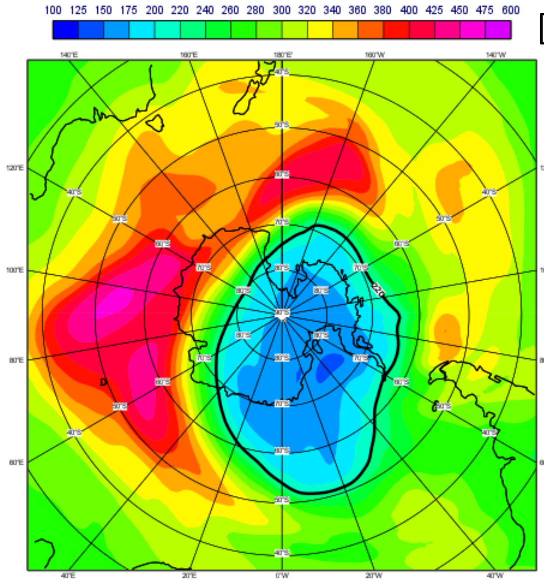
Increment created by a single ozone observation of 375 DU, 10 DU higher than background

Standard deviation from the background matrix at the observation location

Formulation of the B-matrix is very important for AC

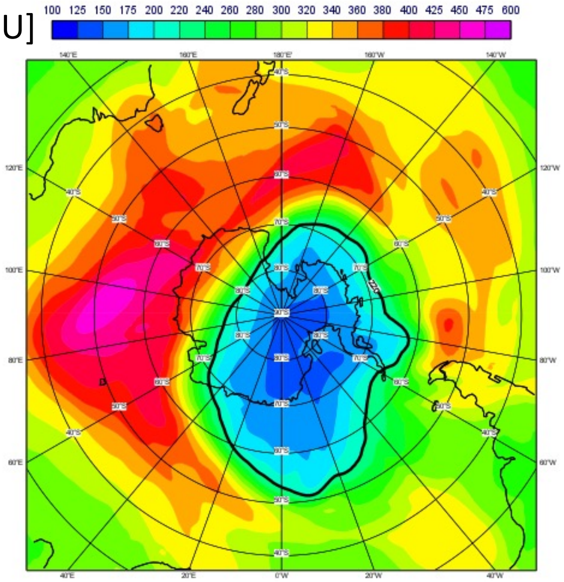
An extreme example: Ozone 7 October 2004

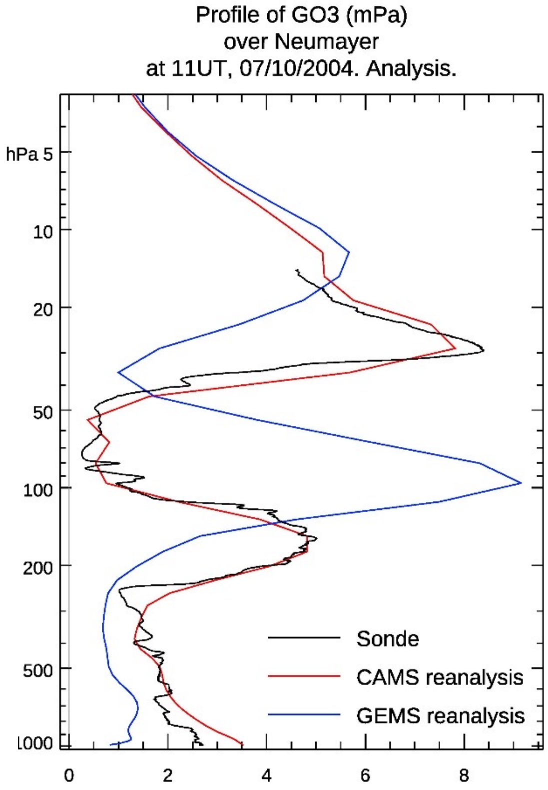
GEMS reanalysis



[DU]

CAMS reanalysis





Sonde launched by AWI

- Similar TCO3 analysis from (old) GEMS reanalysis and CAMS reanalysis
- Huge differences between corresponding O3 profiles
- No profile data (MIPAS, MLS) were assimilated in GEMSRA in Oct 2004 and model had a large O3 bias leading to very bad vertical O3 analysis profiles
- Shows importance of using limb sounding data for O3 analysis

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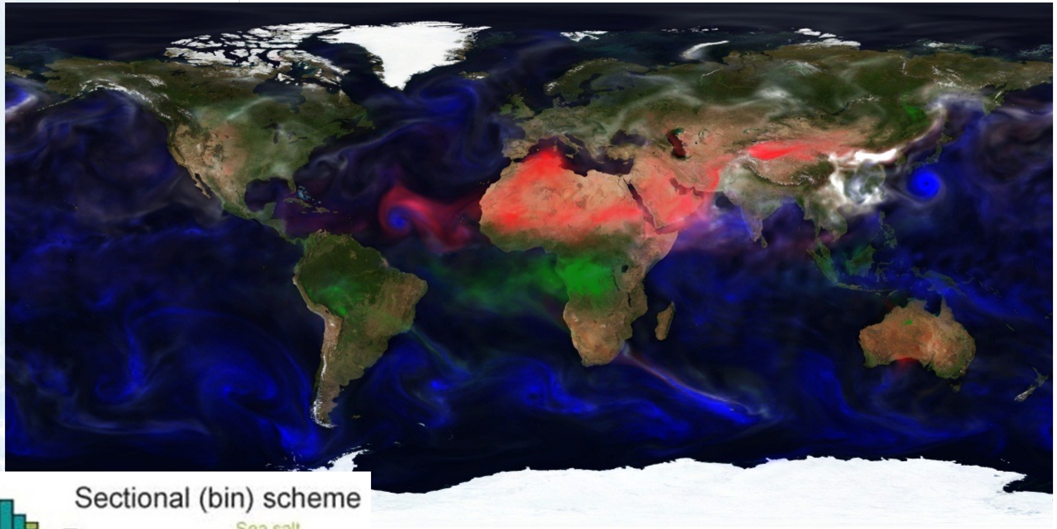
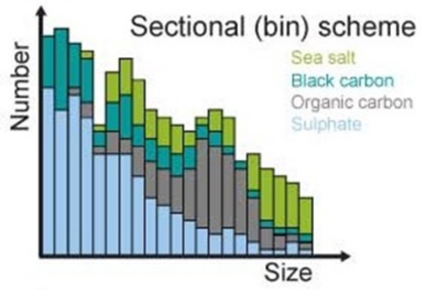
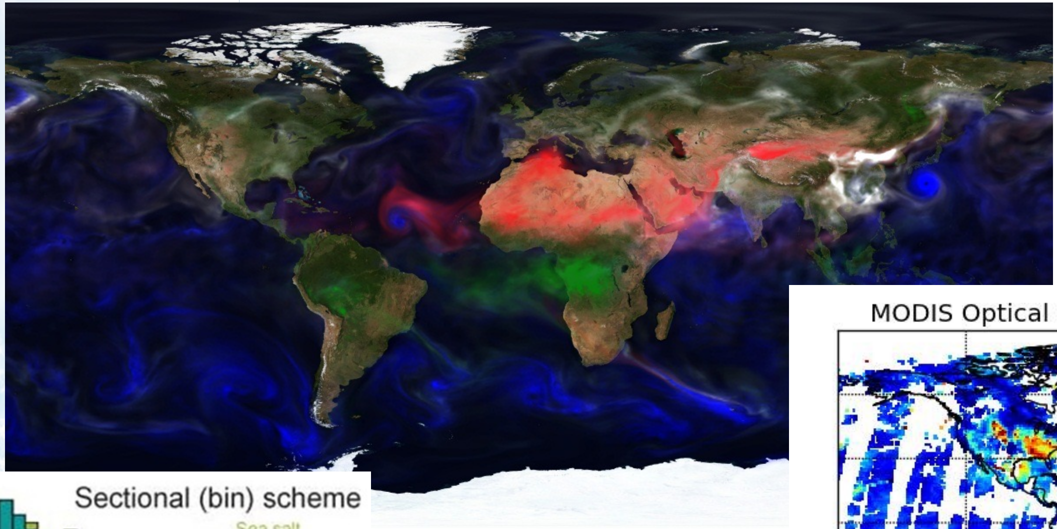
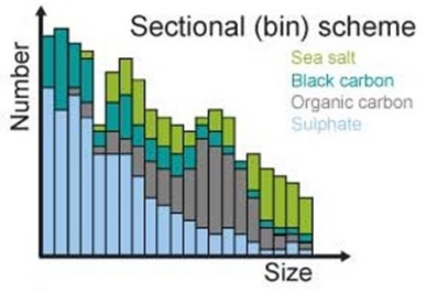
Aerosol – an ill-observed system

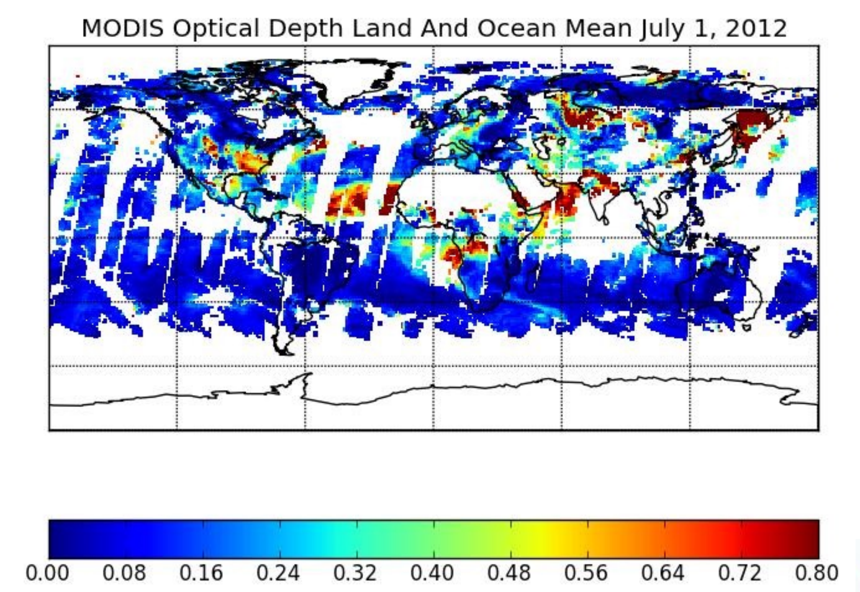




Aerosol – an ill-observed system



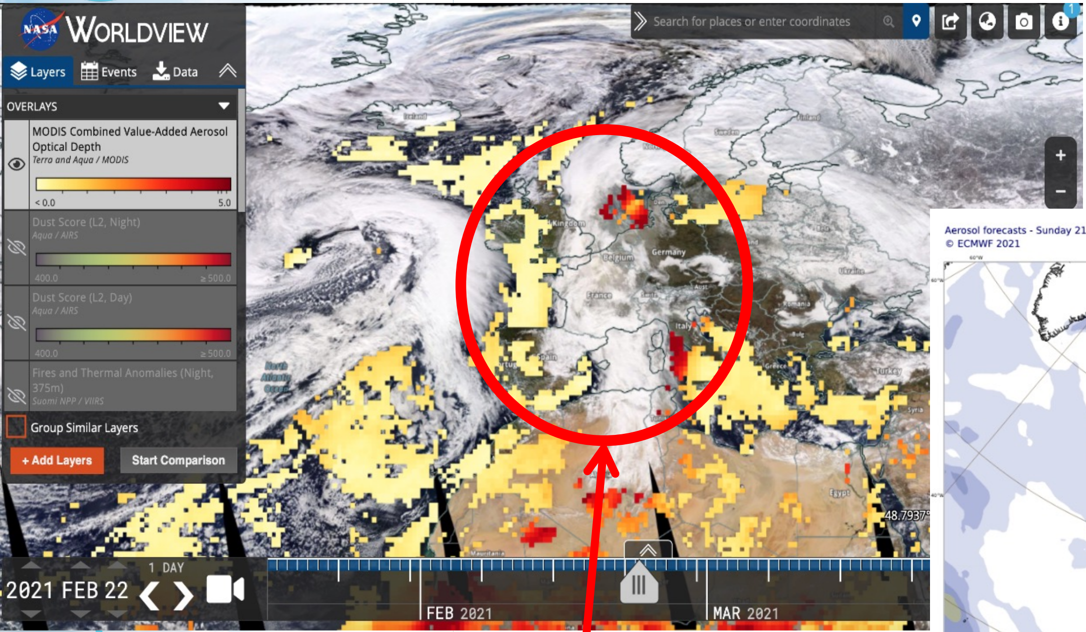




Aerosol analysis

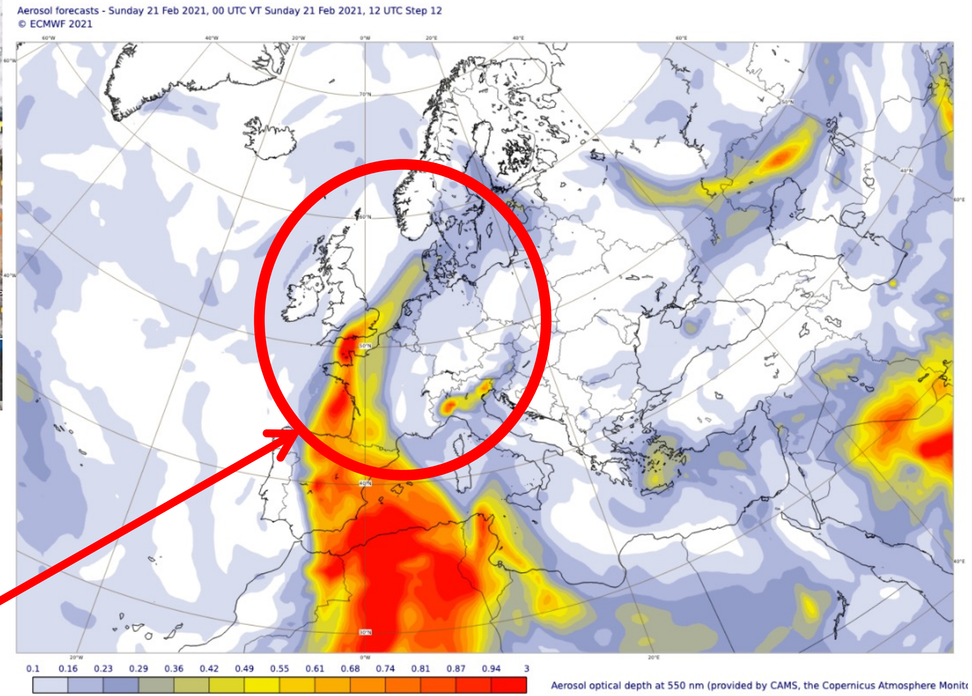
- CAMS aerosol model has 16 aerosol bins:
  - 3 size bins each for sea-salt and desert dust
  - 2 bins (hydrophilic and hydrophobic) each for organic matter and black carbon
  - 1 bin for sulphate
  - 2 bins (fine and coarse) for nitrate
  - 1 bin for ammonium
  - 2 bins for SOA
- Assimilated observations are AOD at 550 nm from MODIS (Aqua and Terra) and VIIRS (SNPP and NOAA20) over land and ocean & PMAp (Metop-BC) over ocean
- Control variable is formulated in terms of the total aerosol mixing ratio.
- Analysis increments are repartitioned into the species according to their fractional contribution to the total aerosol mixing ratio.
- The repartitioning of the total aerosol mixing ratio increment into the different bins is difficult

Dust storm February 2021



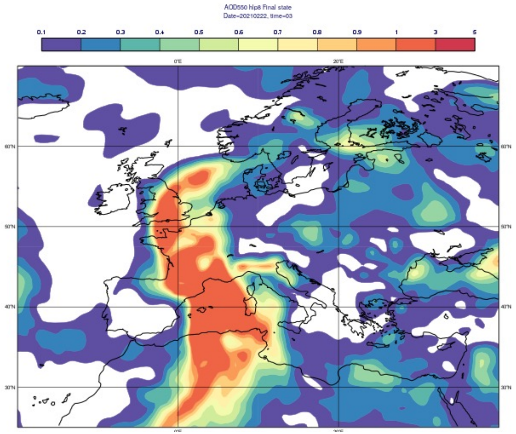
NASA Worldview – MODIS Aqua and Terra AOD 550nm observations for 20210222

CAMS Total AOD at 550nm 12hr forecast valid at 20210222 12hr



The CAMS forecast does a good job of forecasting the AOD plume from Africa over Northern Europe

Dust test case February 2021



Total AOD at 550nm: 20210222 03hr

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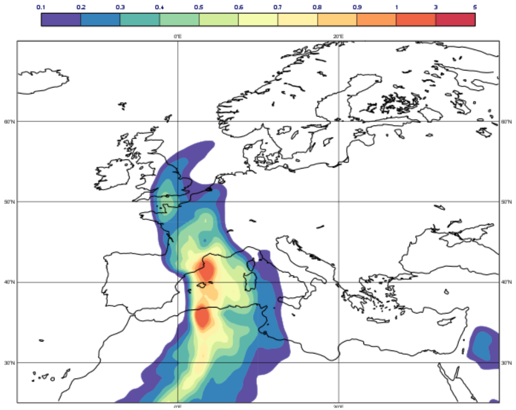
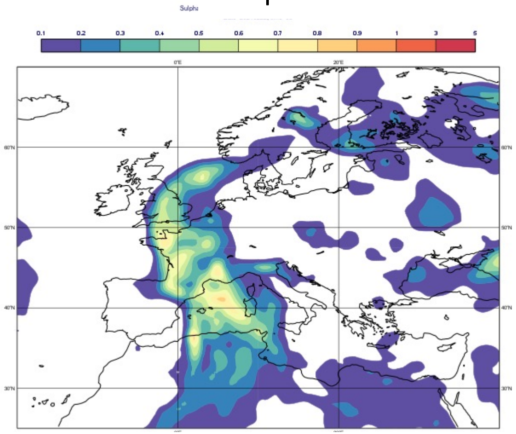
Dust

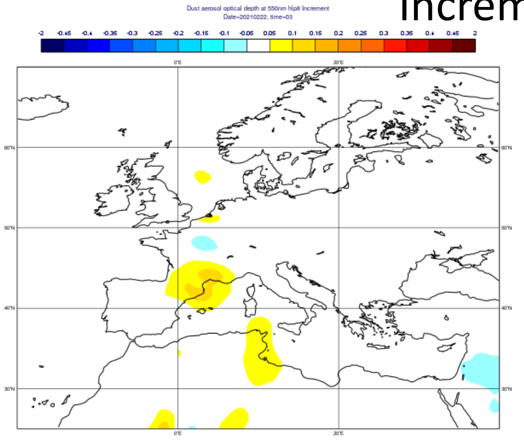


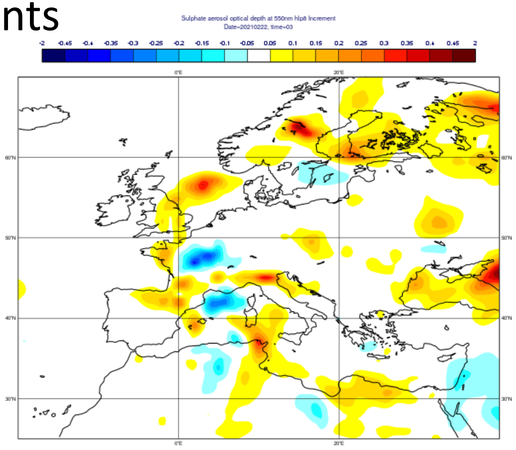
Sulphate



AOD at 550nm

Increments



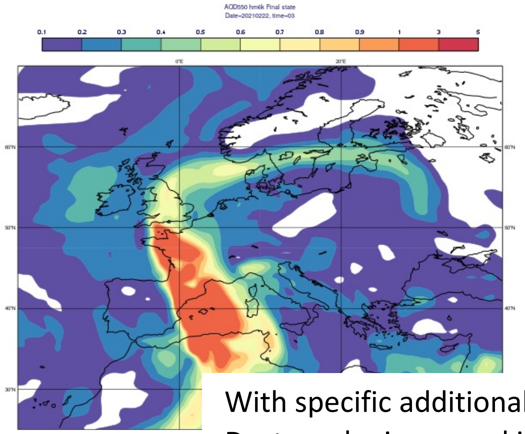


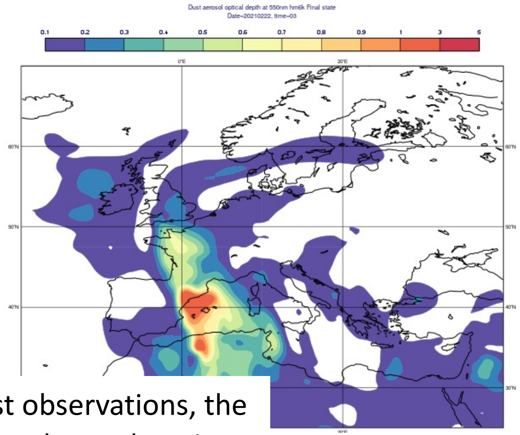
AOD incr at 550nm

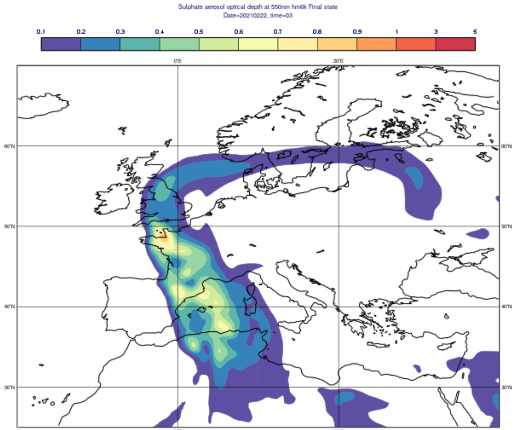
- AOD increments are attributed to the different species according to their proportion in the nonlinear forecast.
- If there is no dust in the forecast in a specific location then the increment will be given to whatever species are there – in this case Sulphate

European Commission

Dust test case February 2021

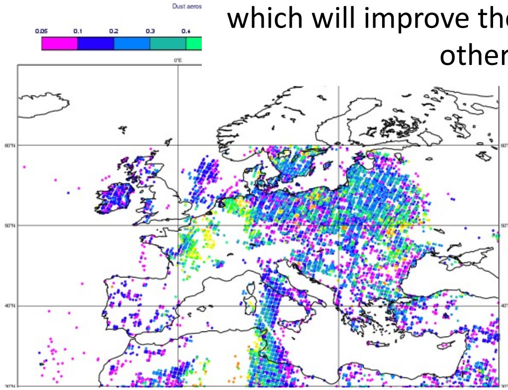




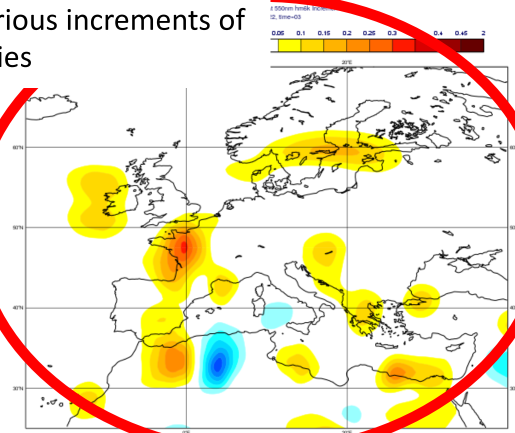


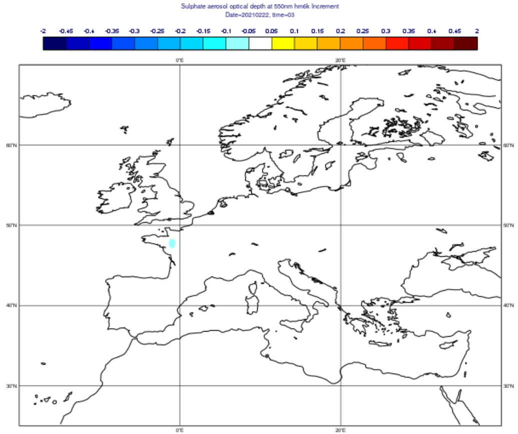
AOD at 550nm

With specific additional Dust observations, the Dust can be increased in the relevant locations which will improve the spurious increments of other species



LMD IASI 10um obs 20210222 12hr





AOD incr at 550nm

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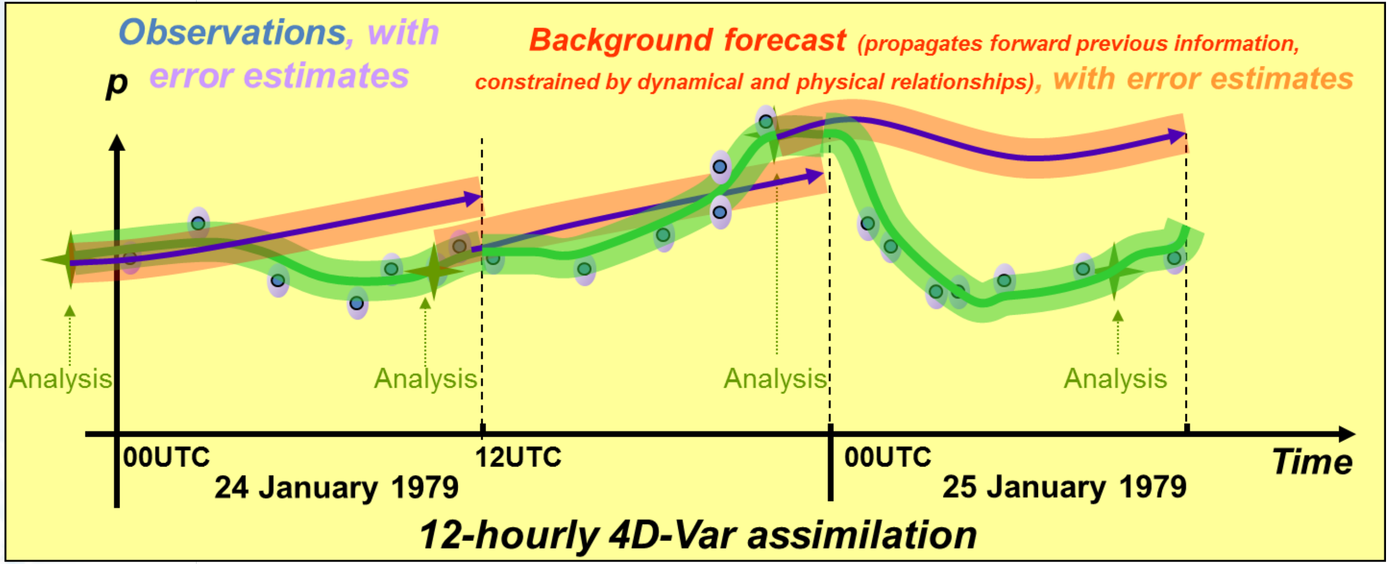
5. Emissions and emission inversion

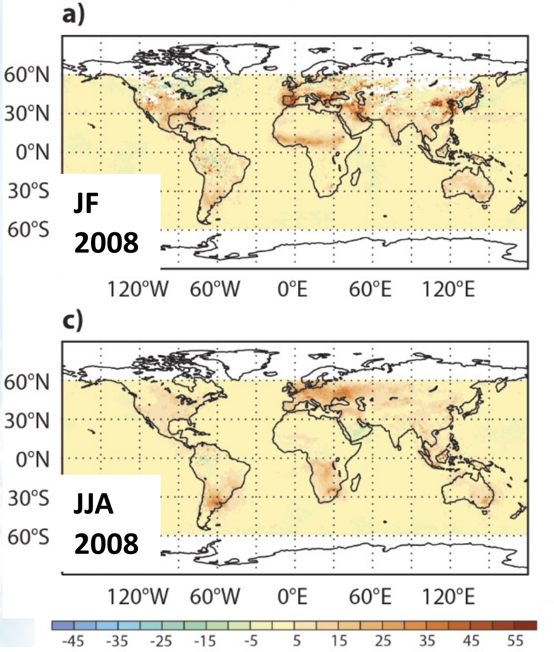
Initial condition vs boundary problem



- NWP 4D-Var is mostly defined as an initial value problem. Only initial conditions are changed and model error is relatively small.
- AC modelling depends on initial state and surface fluxes
- Large part of chemical system not sensitive to initial conditions because of chemical equilibrium, but dependent on other parameters (e.g. emissions, deposition, reaction rates, …) which all might have errors

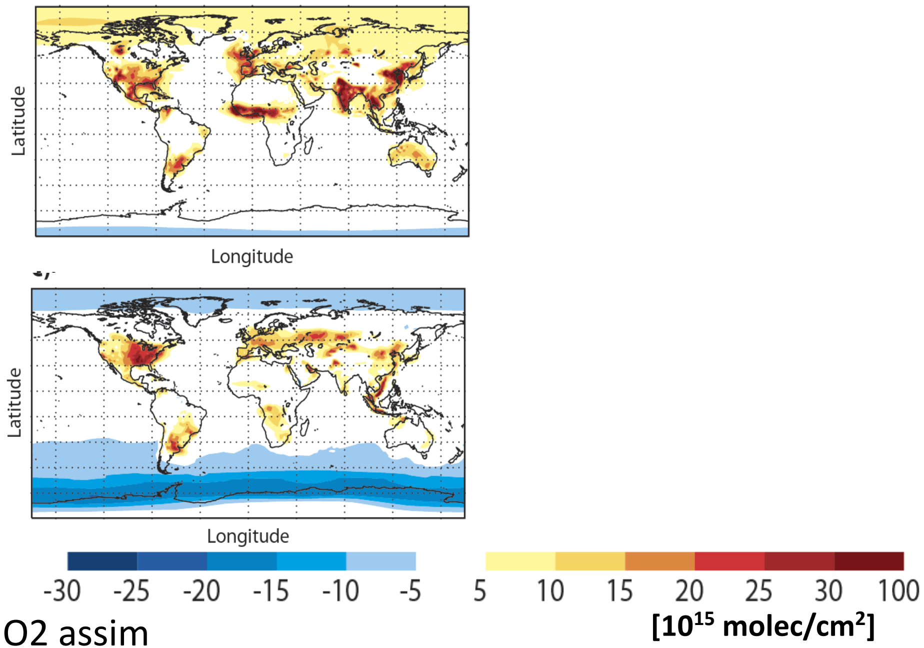
Short-lived memory of NO2 assimilation

OMI NO2 analysis increment [%]



Differences between

Assim and CTRL



- Large positive increments from OMI NO2 assim
- Large differences between analyses of ASSIM and CTRL

Inness et al. (2015, ACP)

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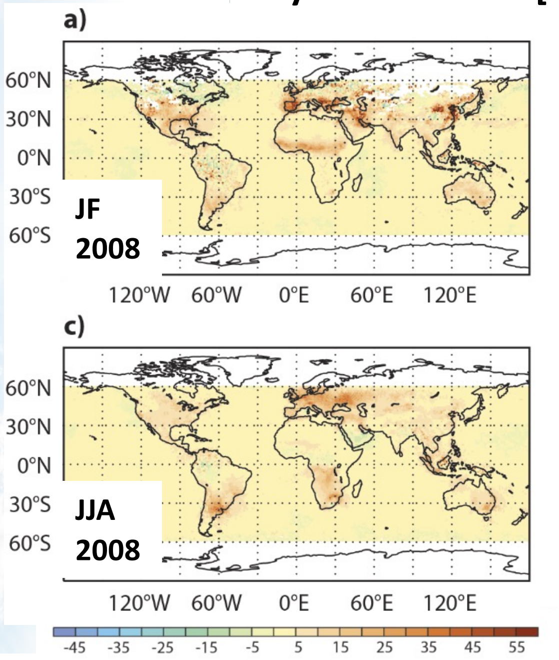
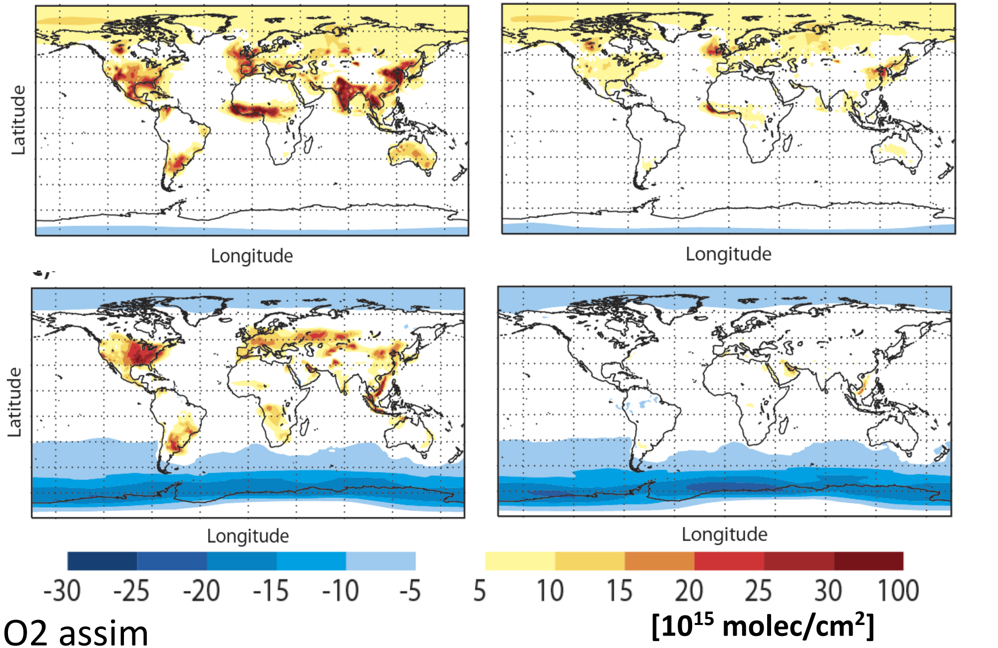
Short-lived memory of NO2 assimilation

OMI NO2 analysis increment [%]



Differences between Assim and CTRL

Difference between 12h forecasts from ASSIM and CTRL



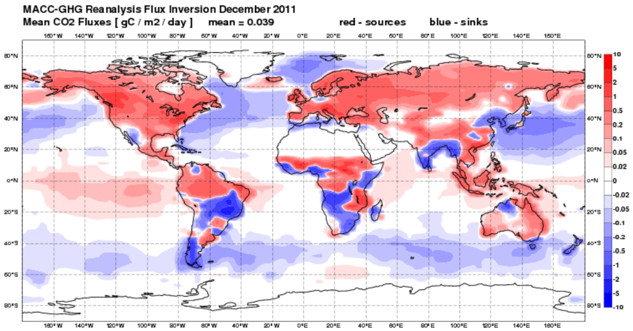
- Large positive increments from OMI NO2 assim
- Large differences between analyses of ASSIM and CTRL
- Impact is lost during subsequent 12h forecast
- Constraining emissions (in addition of IC) would give a better initial state and persistence of forecast improvements throughout the DA window

Inness et al. (2015, ACP)

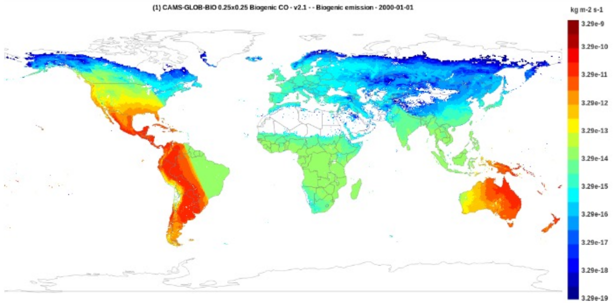
Examples of emissions

TNO European anthropogenic NOx emissions

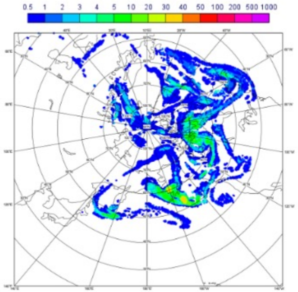
CO2 fluxes



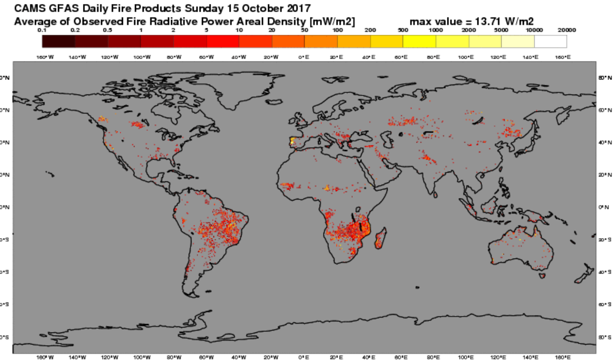
CAMS_GLOB biogenic CO emissions



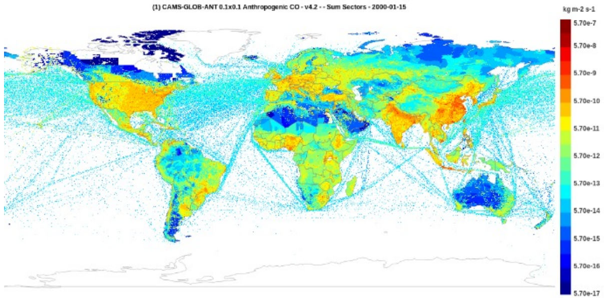
Volcanic SO2



Biomass burning, 15 October 2017



CAMS_GLOB anthropogenic emissions



Emissions

- Emissions are one of the major uncertainties in composition modeling (can not be measured directly)
- The compilation of emissions inventories is a labour-intensive task based on a wide variety of socio-economic and land use data
- Trends are applied to inventories from previous years to produce future emission datasets
- Some emissions can be "modeled" based on wind (dust and sea salt aerosol) or temperature (biogenic emissions)
- Some emissions can be observed indirectly from satellites instruments (Fire radiative power, burnt area, volcanic plumes)
- "Inverse" methods can be used to correct prior emission estimates using observations of concentrations and models

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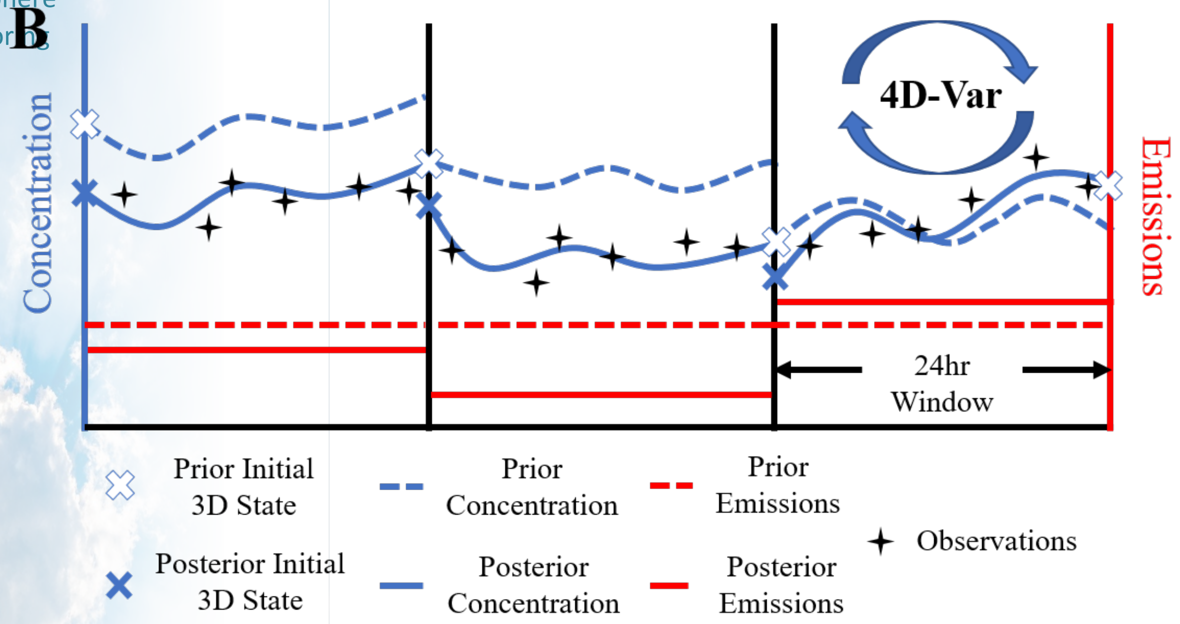
Including emissions in the control vector

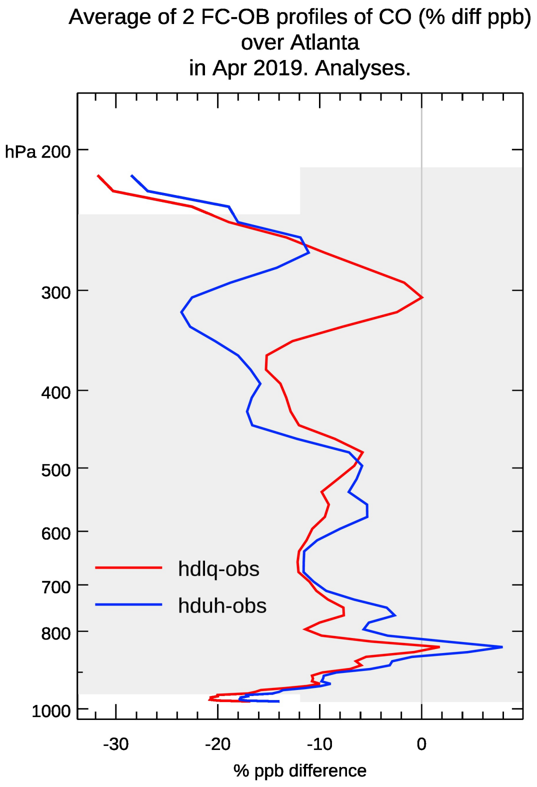


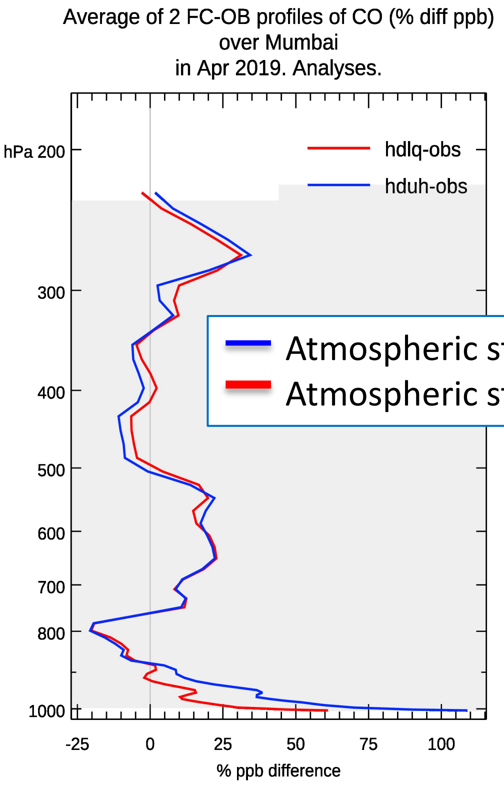
How to improve?

Use the data assimilation system to adjust surface fluxes at the same time as the initial atmospheric conditions.

McNorton, J., Bousserez, N., Agustí-Panareda, A., Balsamo, G., Engelen, R., Huijnen, V., Inness, A., Kipling, Z., Parrington, M., and Ribas, R.: Quantification of methane emissions from hotspots and during COVID-19 using a global atmospheric inversion, Atmos. Chem. Phys. Discuss. [preprint], https://doi.org/10.5194/acp-2021-1056, in review, 2022.

Including emissions improves the forecast





Including emissions in the DA control vector results in significant improvements in modelled CO mixing ratios at the surface and in the upper troposphere.

- Atmospheric state-only (blue)
- Atmospheric state & emissions (red)

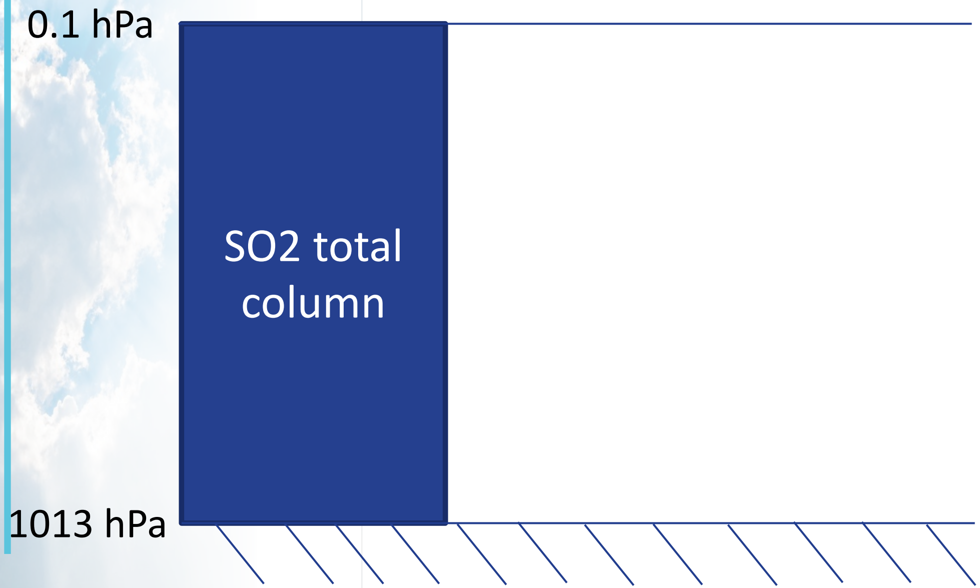
Over Mumbai, emissions are adjusted locally, while Atlanta show the long-range transport effect of adjusted emissions elsewhere.

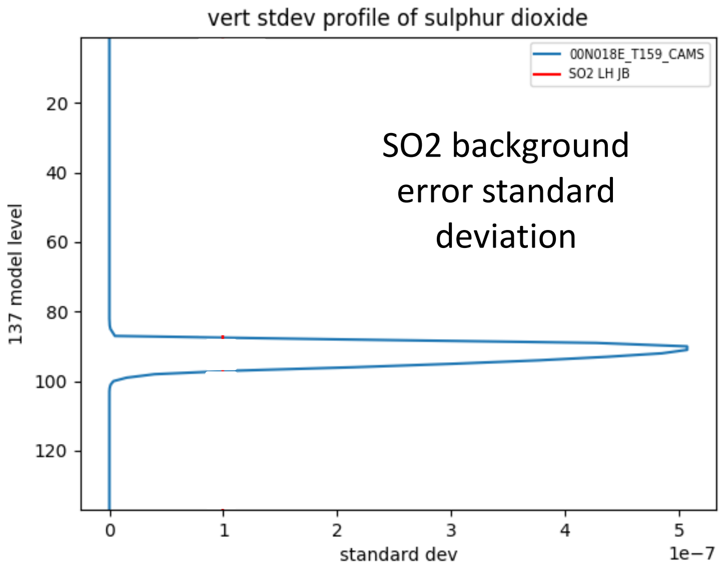
Using observations to create emissions

Atmosphere Monitoring

OLD

- Use of total column SO_2 (0.01-1013 hPa). Averaging kernels currently not used.
- JB peaks at ml=98
- Only volcanic flagged observations used





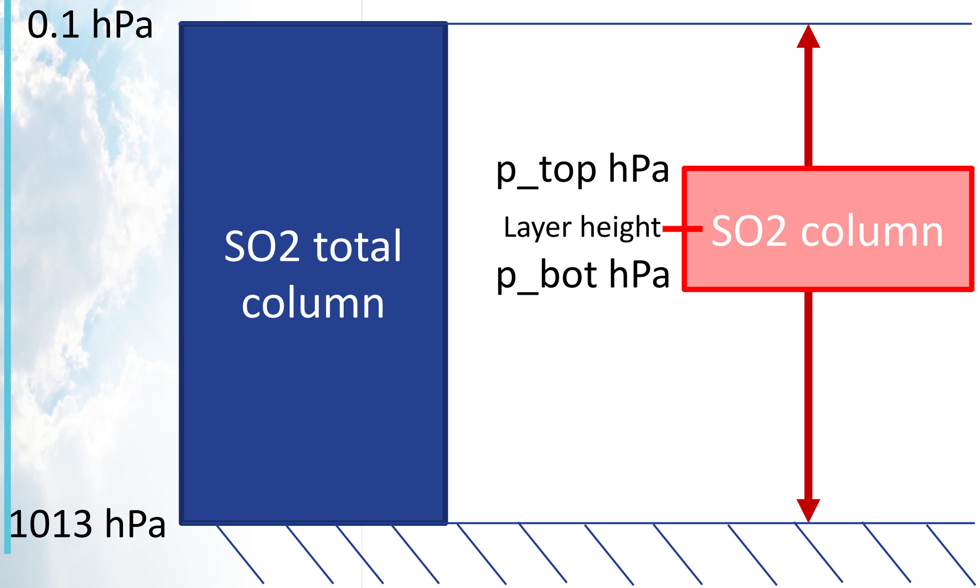
Using observations to create emissions

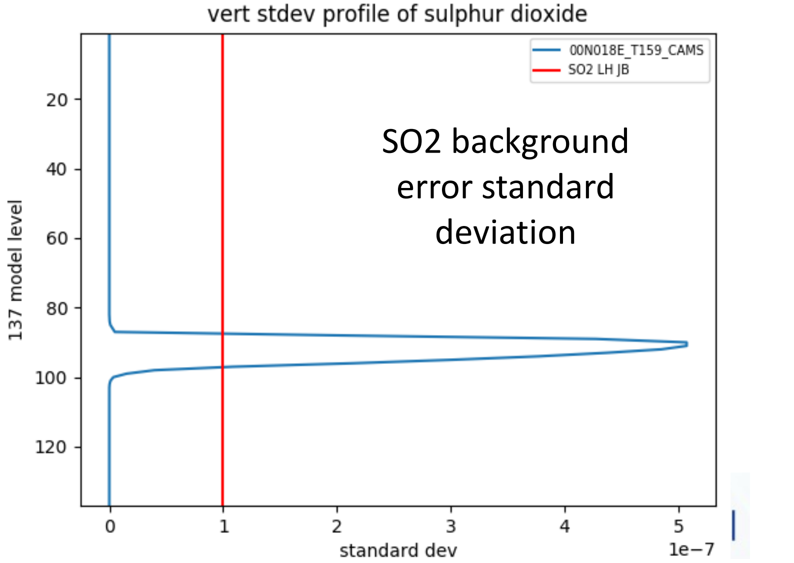
OLD

- Use of total column SO2 (0.01-1013 hPa). Averaging kernels currently not used.
- JB peaks at ml=98
- Only volcanic flagged observations used

NEW

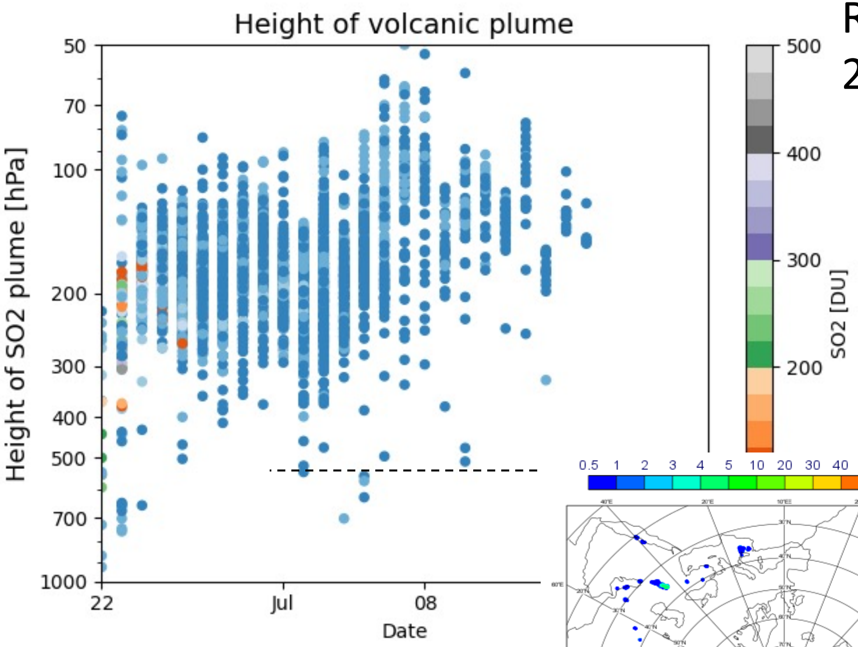
- Use of layer SO2 :
  - p_top=plume_pressure*(1-0.2)
  - p_bot=plume_pressure*(1+0.2)
- Use const background errors, e.g. $1e^{-7}$ kg/kg at all levels

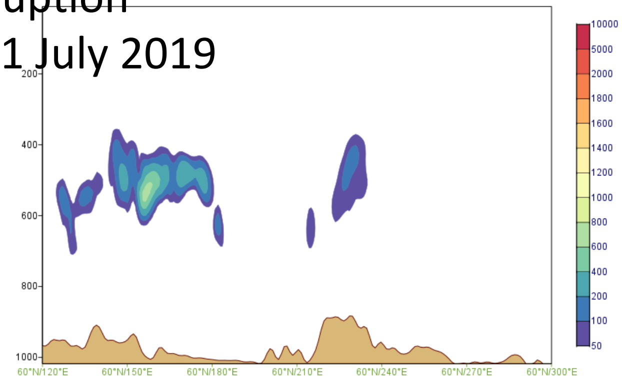




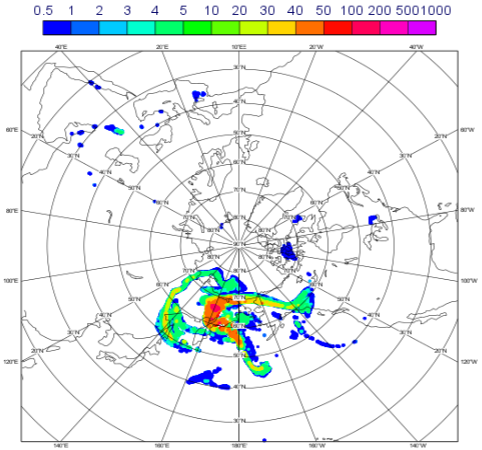
Using observation to create emissions

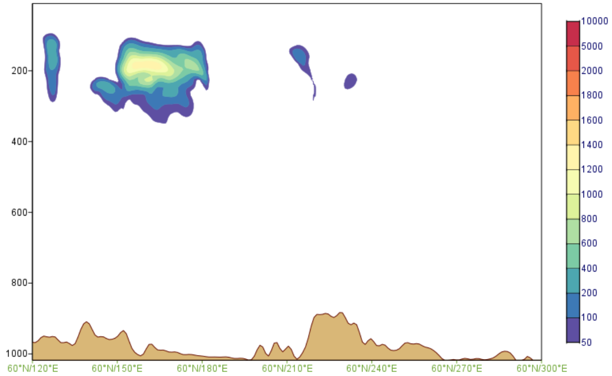
Raikoke eruption
22 June -21 July 2019





Base run





LH exp

Assumption of placing the SO2 signal around 550 hPa is clearly wrong

Atmosphere Monitoring

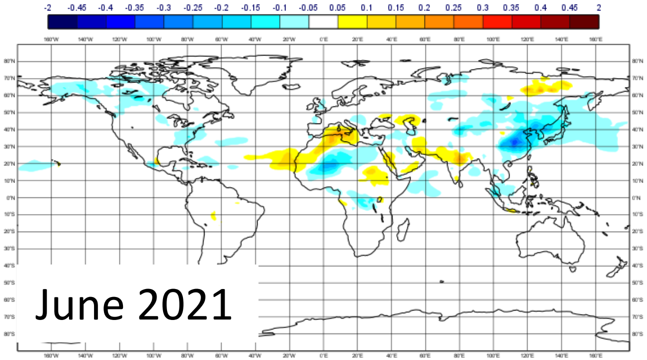
6. Potential benefits for NWP

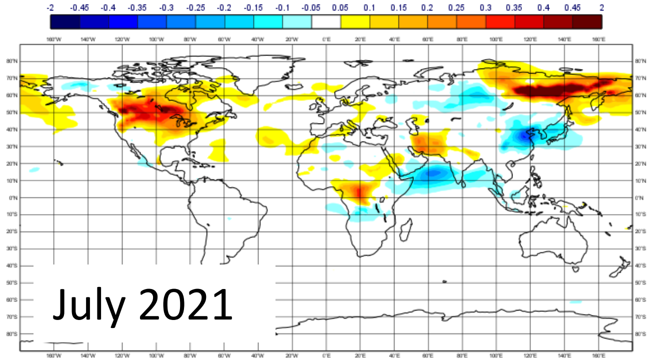
European Commission | ECMWF

Atmosphere Monitoring

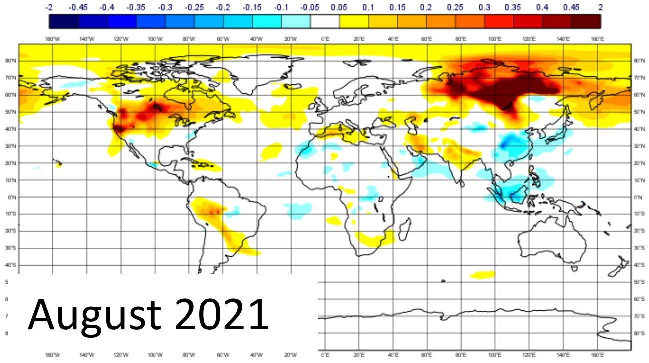
Impact of prognostic aerosols

AOD anomalies and boreal wildfires summer 2021



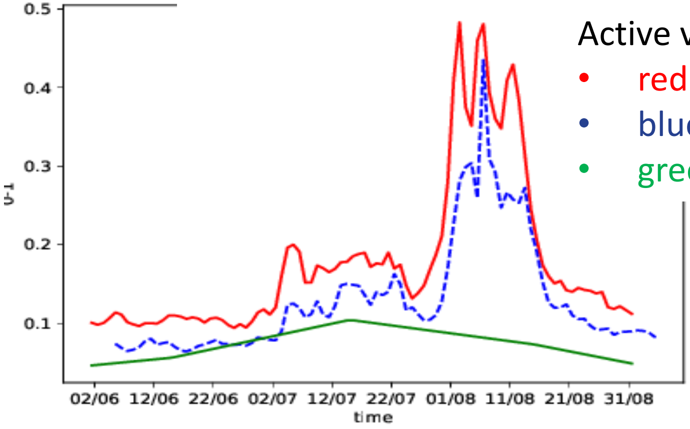


AOD anomalies due to Siberian and N-American wildfires in JJA 2021



Anomalies calculated against 2003-2020 monthly means from CAMS reanalysis

AOD mean Artic JJA 2021



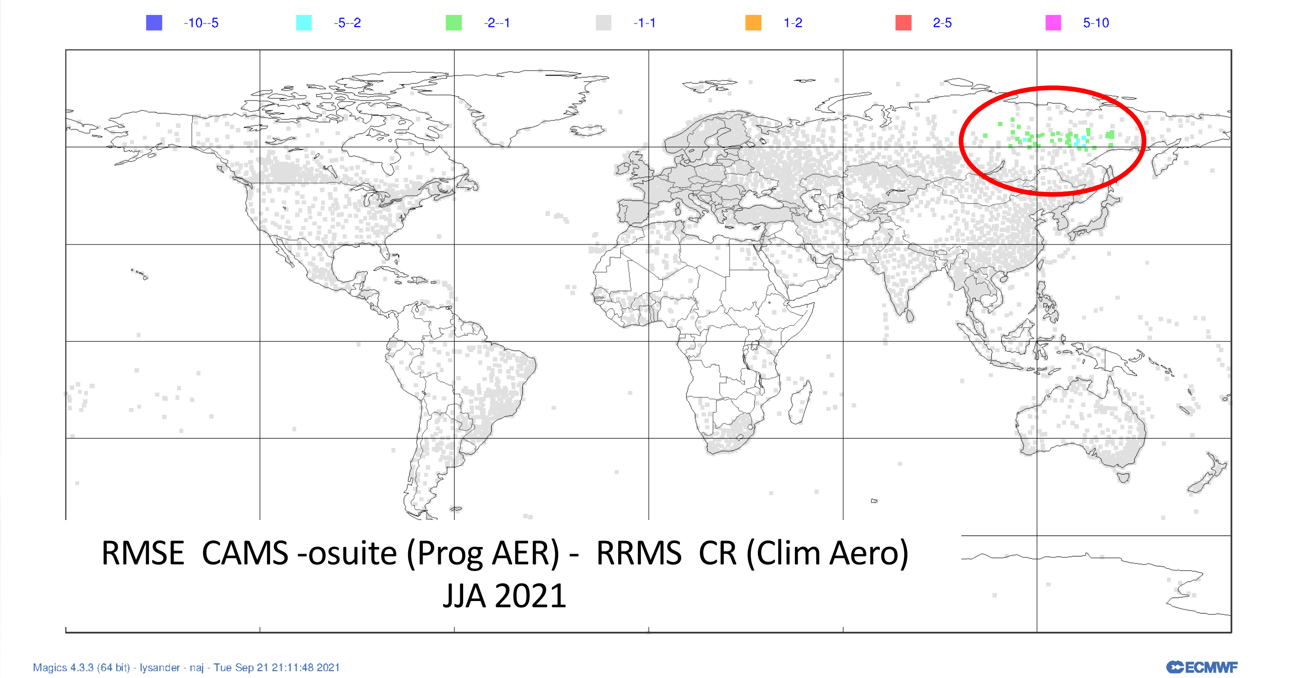
Active vegetation fires in Siberia

- red: AOD analysis,
- blue: 108 h forecast
- green: climatology

Credit: Johannes Flemming

Impact on Artic wildfires on 2m temperature forecasts (JJA 2021)

Atmosphere Monitoring



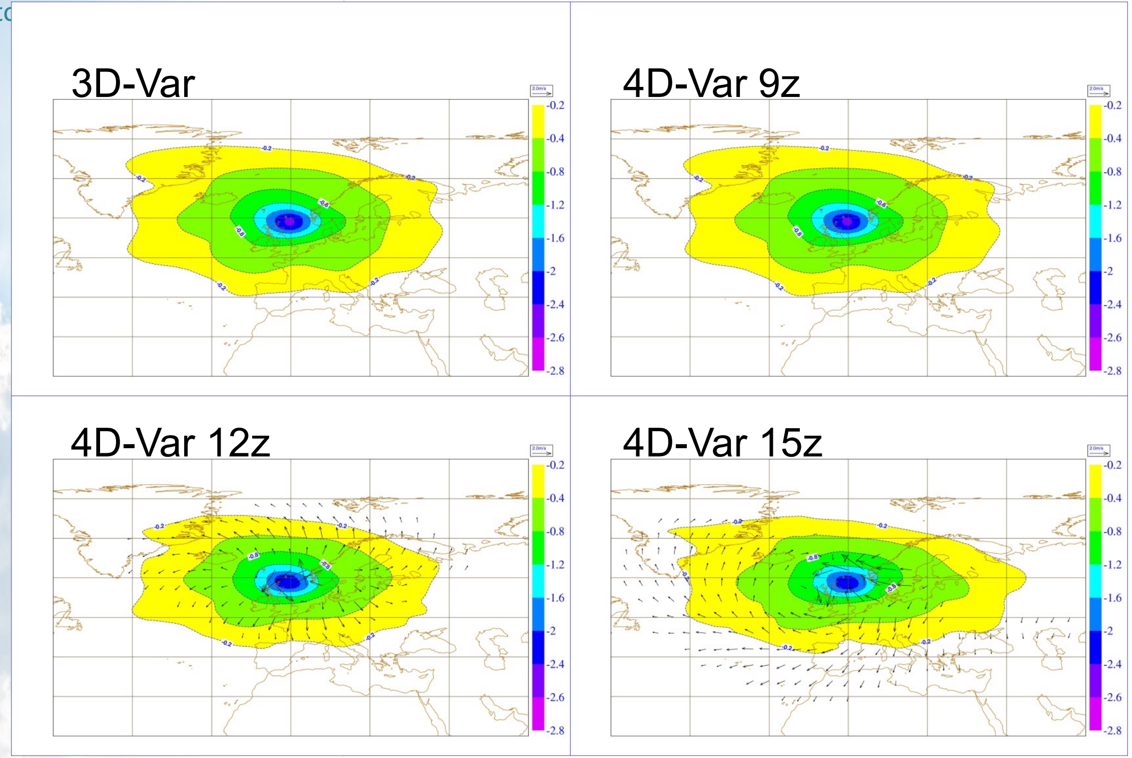
Using prognostic aerosols leads to decrease in 2m temperature RMSE against synop observations

Credit: Johannes Flemming

Wind information from tracers

- Prospect to extract wind information from long lived tracers in stratosphere and upper troposphere, e.g. $O3$, $H2O$, $N2O$.
- Similar to cloud-track winds but data coverage worse.
- Potential was demonstrated in early studies for $H2O$ (Thepaut 1992) and $O3$ (Daley 1995; Riishojgaard 1996; Holm 1999; Peuch et al. 2000)
- Could compliment existing wind observations and help in areas where there is a lack of adequate global wind profile data

Ozone and wind increments



Level 20,
≈ 30 hPa

Observation at T0: 4D-Var = 3D-Var

Observation at T3: wind increments

Observation at T6: wind increments

6h assimilation window

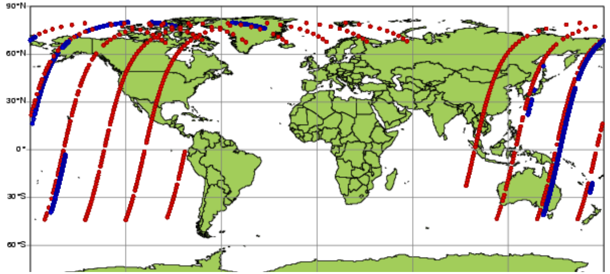
Single observation experiments

Requirements to extract wind info from tracers

Atmosphere Monitoring

- Complete data coverage (3D), frequent observations.
- Accurate observations and high-quality background field
- No bias between observations and background
- Depends on accuracy of TL model compared to full model (better for passive tracers/ long chemical lifetime)
- Studies have looked at this in idealized experiments (e.g. Daley 1995; Riishojgaard 1996; Peuch et al. 2000; Allen et al. 2013, 2014, 2018) focusing on long-lived tracers O3, H2O, N2O and found positive impact for perfect (and frequent) observations.
- Few studies used real data (e.g. MLS O3, Semane et al. 2009) and positive results are less clear for ‘not perfect’ or infrequent observations

Example from ERA-Interim (it went wrong)



GOME 15-layer profiles (~15,000 per day)
SBUV 6-layer profiles (~1,000 per day)

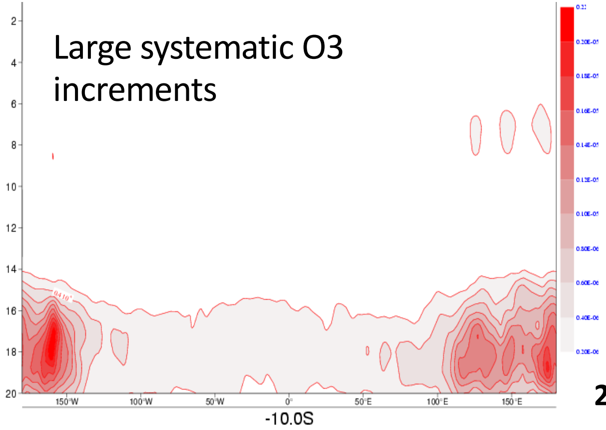
The stratosphere is not well constrained by observations:

- Ozone profile data generate large temperature increments
- 4D-Var adjusts the flow where it is least constrained, to improve the fit to observations

=> IFS O3 analysis is completely uncoupled now

Ozone increments at 10S

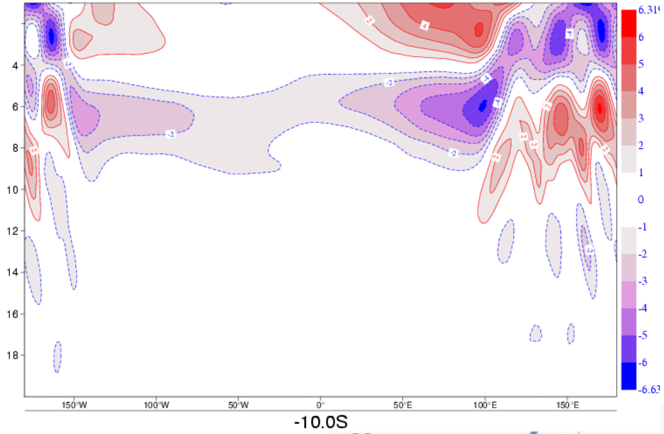
Large systematic O3 increments



1 hPa

20 hPa

Associated Temp increments



D. Dee

Potential benefit for NWP

- Prognostic aerosols, feedback on dynamics via radiation scheme: NWP first used Tegen AER climatology in radiation scheme, then CAMS interim climatology from CY43R3 and CAMSRA climatology from 48R1 onwards. CAMS uses aerosols interactively
- Dynamical coupling with wind/T through TL and AD: turned off
- Use of O3 (& other fields) in the radiation scheme: MACC climatologies used in NWP. CAMS uses interactive O3.
- RTTOV observation operator: Use of O3, CO2 analysis fields to improve the use of radiances sensitive to O3, CO2: model O3 is used, but climatologies used for other tracers (e.g. fixed CO2 value)
- Multivariate JB: Correlations between tracers and dynamical variables, e.g. O3 and vorticity; correlations between chemical species: univariate

Atmosphere Monitoring

7. Summary

Atmosphere Monitoring

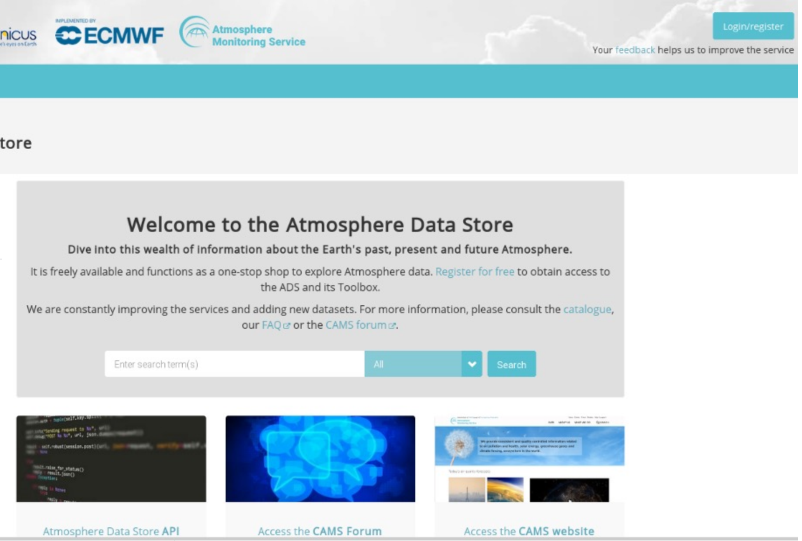
What we have seen today…

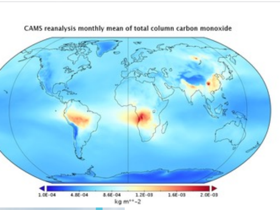
- Basic Data Assimilation theory is the same
- Particular challenges related to DA for atmospheric composition
  - Boundary conditions (emissions) as well as initial conditions; inversions
  - Mismatches between modelled and observed variables
  - Fast reactions and short life-time of some species
- Atmospheric composition has the potential to improve various aspects of NWP
- CAMS produces useful global and regional European Atmospheric Composition forecasts and analyses, freely available from atmosphere.copernicus.eu

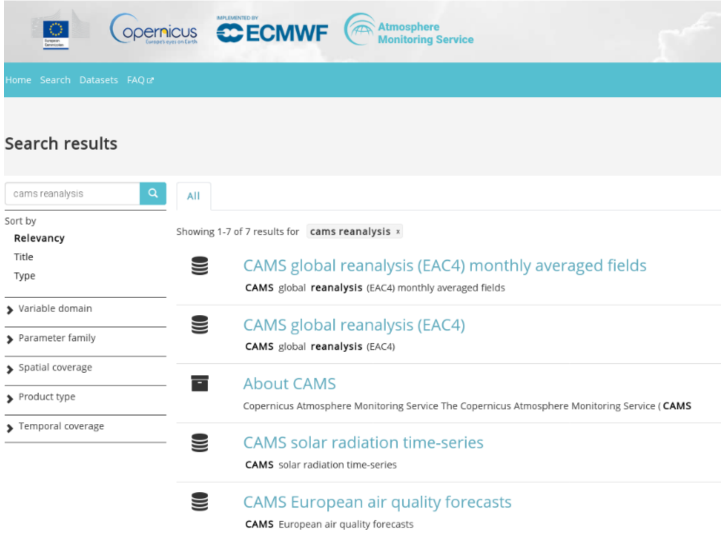
The Atmosphere Data Store (ADS)

Atmosphere Monitoring

All CAMS data are freely available https://atmosphere.copernicus.eu/data







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Atmosphere Monitoring

2. Data assimilation methodology for atmospheric composition

Copernicus Europe's eyes on Earth | European Commission | ECMWF

Cost function

Atmosphere Monitoring

Data assimilation for atmospheric composition is in principle no different from NWP data assimilation

Analysis: x that minimizes cost function

$$J(x) = \underbrace{(x - x_b)^T B^{-1}(x - x_b)}_{J_b} + \underbrace{\sum_{i=0}^{n}(y_i - H_i[x_i])^T R_i^{-1}(y_i - H_i[x_i])}_{J_o}$$

Cost function

J_b
Background term

J_o
Observation term

x: control vector
x_b: model background (short forecast)
B: Background error covariance matrix
y: Observations
H[x]: Model equivalent of observations
R: Observation error covariance matrix

- **Strong constraint 4D-Var** assumes perfect model over assimilation period
- Weak constrained 4D-Var includes a model error term

Data assimilation methodology

Data assimilation for atmospheric composition is in principle no different from NWP data assimilation

$$J(x) = (x - x_b)^T B^{-1} (x - x_b) + \sum_{i=0}^{n} (y_i - H_i[x_i])^T R_i^{-1} (y_i - H_i[x_i])$$

Control variables

NWP

vorticity
divergence
temperature
surface pressure (logarithm)
specific humidity

Atmospheric Composition

ozone
carbon monoxide
nitrogen dioxide
formaldehyde
sulphur dioxide

carbon dioxide
methane

aerosol mixing ratio

IFS

Atmosphere Monitoring

Data assimilation methodology

Data assimilation for atmospheric composition is in principle no different from NWP data assimilation

$$J(x) = (x - x_b)^T B^{-1}(x - x_b) + \sum_{i=0}^{n}(y_i - H_i[x_i])^T R_i^{-1}(y_i - H_i[x_i])$$

Control variables

NWP

vorticity
divergence
temperature
surface pressure (logarithm)
specific humidity

Atmospheric Composition

ozone
carbon monoxide
nitrogen dioxide
formaldehyde
sulphur dioxide

carbon dioxide
methane

aerosol mixing ratio

Chemical module

GHG module

Aerosol module

Chemical Module IFS

TM5 (CB05)
57 species, 131 reactions
Photolysis, dry and wet deposition

ECMWF Copernicus Europe's eyes on Earth European Commission

Data assimilation methodology

Data assimilation for atmospheric composition is in principle no different from NWP data assimilation

$$J(x) = (x - x_b)^T B^{-1} (x - x_b) + \sum_{i=0}^{n} (y_i - H_i[x_i])^T R_i^{-1} (y_i - H_i[x_i])$$

Control variables

NWP

vorticity
divergence
temperature
surface pressure (logarithm)
specific humidity

Atmospheric Composition

ozone
carbon monoxide
nitrogen dioxide
formaldehyde
sulphur dioxide

carbon dioxide
methane

aerosol mixing ratio

Chemical module

GHG module

Aerosol module

IFS

Greenhouse Gas Module

CHTESSEL
Photosynthesis & ecosystem respiration model
Diagnoses the gross primary production of CO_2 by plants and release of CO_2 by soil

CH_4 comes from prescribed emissions and climatological loss

Atmosphere Monitoring

Data assimilation methodology

Data assimilation for atmospheric composition is in principle no different from NWP data assimilation

$$J(x) = (x - x_b)^T B^{-1} (x - x_b) + \sum_{i=0}^{n} (y_i - H_i[x_i])^T R_i^{-1} (y_i - H_i[x_i])$$

Control variables

NWP

vorticity
divergence
temperature
surface pressure (logarithm)
specific humidity

Atmospheric Composition

ozone
carbon monoxide
nitrogen dioxide
formaldehyde
sulphur dioxide

carbon dioxide
methane

aerosol mixing ratio

IFS

Chemical module

GHG module

Aerosol module

Aerosol bin scheme

14 aerosol-related prognostic variables:
3 bins sea-salt, 3 bins dust, Black carbon, Organic matter, Sulphate,
2 bins Nitrate, Ammonium

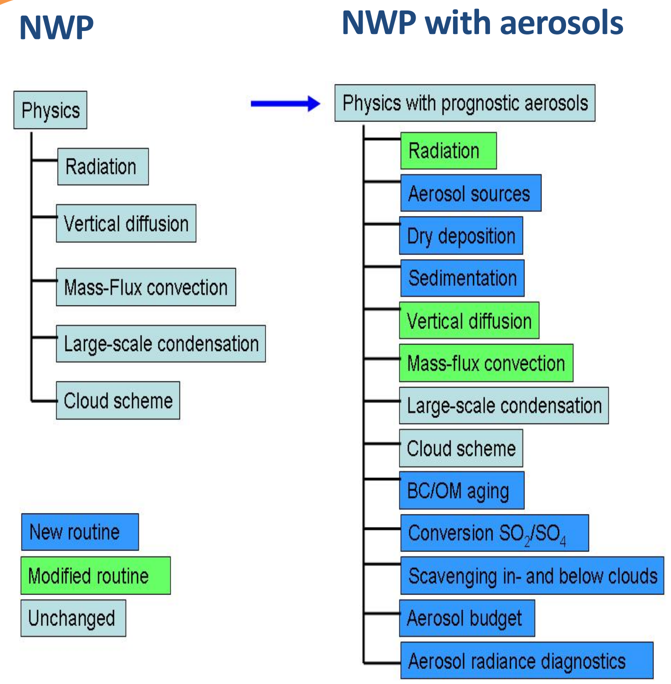
Emissions, dry and wet deposition, sedimentation

Combining the AC and NWP models

- Atmospheric composition models can be run coupled to NWP or fully integrated.

IFS

In the IFS the atmospheric composition and NWP models are fully integrated



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Data assimilation methodology

$$J(\delta \mathbf{x}) = \frac{1}{2}\delta \mathbf{x}^{\mathrm{T}}\mathbf{B}^{-1}\delta \mathbf{x} + \frac{1}{2}\sum_{i=0}^{n}(\mathbf{H}_i\delta \mathbf{x}(t_i) - \mathbf{d}_i)^{\mathrm{T}}\mathbf{R}_i^{-1}(\mathbf{H}_i\delta \mathbf{x}(t_i) - \mathbf{d}_i)$$

Resolutions of CAMS NRT system